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Computational Experimentation

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ABSTRACT

Experimentation conjures images of laboratories and equipment in biotechnology, chemistry, materials science, and pharmaceuticals. Yet modern day experimentation is not limited to only chemical synthesis, but is increasingly computational. Researchers in the unpredictable arts can experiment upon the functions, properties, reactions, and structures of chemical compounds with highly accurate computational techniques. These computational capabilities challenge the enablement and utility patentability requirements. The patent statute requires that the inventor explain how to make and use the invention without undue experimentation and that the invention have at least substantial and specific utility. These patentability requirements do not align with computational research capabilities, which allow inventors to file earlier patent applications, develop prophetic examples, and provide supporting disclosure in the patent specification without necessarily conducting traditional, laboratory-based experiments. This Article explores the contours and applications of computational capabilities on patentability, proposes reforms to the utility doctrine and to patent examination, responds to potential critiques of the proposed reforms, and analyzes innovation policy in the unpredictable arts. In light of increasing computational experimentation, this Article recommends strengthening the utility requirement in order to prevent a state of patent law in which enablement is subsumed into utility.

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I. INTRODUCTION

To invent, you need a good imagination and a pile of junk.
– Thomas Edison

Thought experiment is in any case a necessary precondition for physical experiment. Every experimenter and inventor must have the planned arrangement in his head before translating it into fact.
– Ernst Mach

Computational research and development is displacing laboratory research techniques in the unpredictable arts,[1] which have traditionally required chemical synthesis and physical experiments. Before the advent of computational science tools,[2] researchers in engineering and sciences could only conduct experiments in the physical and tangible world. Inventors traditionally utilized apparatuses, chemicals, consumables, equipment, hardware, instrumentation, measurement tools, reagents, and tangible items to support or validate a hypothesis. Such traditional experiments yielded discoveries for inventors during actual reduction to practice[3] or constructive reduction to practice.[4] This Article suggests that computational research development, which also enables discoveries during conception,[5] challenges the enablement and utility doctrines in US patent law.

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1. *See, e.g.*, Sean B. Seymore, *Heightened Enablement in the Unpredictable Arts*, 56 UCLA L. REV. 127, 137–39 (2008) [hereinafter Seymore, *Heightened Enablement*] (discussing chemistry and experimental sciences as examples of the unpredictable arts, where results are often uncertain, unpredictable, and unexpected; suggesting that embodiments in the unpredictable arts either cannot be made or may require experimentation that is unduly extensive; discussing that the judiciary has recognized the unique challenges that the unpredictable arts bring to the US patent system, yet has struggled to adapt patent law to meet those challenges).

2. Nia Alexandrov & Vassil Alexandrov, *Computational Science Research Methods for Science Education at PG Level*, 51 PROCEDIA COMPUTER SCI. 1685, 1686, 1688–89 (2015) (defining computational science as an interdisciplinary field that melds basic sciences, mathematics, modeling, quantitative analysis techniques, algorithms, parallel programming, and high-performance computing techniques for creating accurate models of coupled physical and biochemical systems).

3. Scott v. Finney, 34 F.3d 1058, 1063 (Fed. Cir. 1994) (necessitating that the invention must have been sufficiently tested that it will work for its intended purpose); Wetmore v. Quick, 536 F.2d 937, 942 (C.C.P.A. 1976) (requiring a showing of the invention in a physical or tangible form).

4. Mark A. Lemley, *Ready for Patenting*, 96 B.U. L. REV. 1171, 1178 (2016) (defining constructive reduction to practice as filing of an enabling patent application).

5. *Id.* at 1177 (explaining that "conception of an invention does not require that the inventor know that the invention will work for its intended purpose," and that conception does not require reduction to practice nor experimentation); Sean B. Seymore, *Serendipity*, 88 N.C. L. REV.

The rise of new computational techniques and rapid increases in computing power allow researchers to conduct experiments *in silico*.[6] Research and development has been changing since computational techniques began allowing engineers and scientists to reduce discovery time and quickly enable numerous discoveries. Computational chemistry,[7] chemoinformatics,[8] computer-aided drug design,[9] protein

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185, 190-191, 201 (2009) [hereinafter Seymore, *Serendipity*] (defining conception as when the inventor formulates a complete idea of the invention, but also noting that this timing is somewhat tricky since conception is a technical inquiry; providing as an example, in the case of a chemical compound, conception does not occur until the inventor has a mental picture of the chemical structure or can sufficiently distinguish it).

6. Le Anh Vu, Phan Thi Cam Quyen & Nguyen Thuy Huong, In silico *Drug Design: Prospective for Drug Lead Discovery*, 4 INT'L J. ENGINEERING SCI. INVENTION 60, 60, 62, 69 (2015) (defining "*in silico*" to mean "computer aided," or using computational environments as their experimental laboratories; providing as an example, "*in silico* drug design," to refer to the rational design by which drugs are designed or discovered by computational methods); *What is* 'In Silico' *Experimentation?*, APACHE TAVERNA [hereinafter TAVERNA], https://taverna.incubator.apache.org/introduction/what-is-in-silico-experimentation [https://perma.cc/3Y2T-UFHG] (last visited Jan. 15, 2019) (defining "*in silico*" experimentation as research conducted via computer simulations with models that closely reflect the real world). The phrase "*in silico*" was coined in 1989 as an analogy to the Latin phrases *in vivo*, *in vitro*, and *in situ*. Vu, Quyen & Huong, *supra*, at 62. Significant advantages of *in silico* experimentation include "higher precision and better quality of experimental data; better support for data-intensive research and access to vast sets of experimental data generated by scientific communities; more accurate simulations through more sophisticated models; faster individual experiments; [and] higher work productivity." *See* TAVERNA, *supra*.

7. ERROL G. LEWARS, COMPUTATIONAL CHEMISTRY: INTRODUCTION TO THE THEORY AND APPLICATIONS OF MOLECULAR AND QUANTUM MECHANICS 1–5 (2d ed. 2011) (defining computational chemistry as "a set of techniques for investigating chemical problems on a computer," including studies of molecular geometry, energies of molecules and transition states, chemical reactivity, chemical spectra, semiempirical calculations based on the Schrödinger equation, and density functional calculations; suggesting that computational chemistry is valuable in the study of properties in materials science and is cheap compared to experiments; and suggesting that computational chemistry simulates the behavior of real physical entities, such that models improve the behavior of atoms and molecules in the real world).

8. Jaroslaw Polanski, *Chemoinformatics*, *in* COMPREHENSIVE CHEMOMETRICS: CHEMICAL AND BIOCHEMICAL DATA ANALYSIS 459, 460, 463, 473 (Steven D. Brown et al. eds., 2009) (defining chemoinformatics as the discipline for the application of computers in chemistry; providing other sources that define chemoinformatics as "the application of informatics methods to solve chemical problems," "the combination of all the information resources that a scientist needs to optimize the properties of a ligand to become a drug," or "emcompass[ing] the design, creation, organization, storage, management, retrieval, analysis, dissemination, visualization and use of chemical information").

9. Gregory Sliwoski et al., *Computational Methods in Drug Discovery*, 66 PHARMACOLOGICAL REV. 334, 336 (2014) (defining Computer Aided Drug Design, or CADD, as either structure-based method involving ligand-docking, pharmacophore, and ligand design methods, or ligand-based methods utilizing "ligand information for predicting activity depending on its similarity/dissimilarity to previously known active ligands").

folding,[10] and nanomaterial rational design[11] increasingly rely upon computational experimentation to predict the chemical functions, properties, reactions, and structures of chemical compounds with high accuracy in advance of, or in conjunction with, chemical synthesis.[12]

To illustrate, consider the following hypothetical: Suppose a researcher-inventor seeks to address the problem of designing optimal pore size chemicals for hazardous gas separation inside of gas masks. Although the researcher-inventor can file a patent application after running a few synthetic chemistry experiments in a laboratory to describe how to make and use the carbon-based particles or other nanomaterials, understand effective chemical treatments and absorptive properties, and provide data from successful use in human subjects that represent test battle conditions, the researcher-inventor may not know with enough certainty how or why certain purities work and how to tune the particles' porosities. It is unknown, for example, if the absorptive activity is due to the combined effect of two or more particular molecules in the nanomaterial. While traditional, time-consuming, and iterative laboratory experiments may determine sufficient details and examples to satisfy current enablement and utility requirements in US patent law, the use of computational techniques could quickly yield prophetic chemical structures[13] with hypothetical properties.[14] The researcher-inventor can run

10. John R. Gunn, *Computational Protein Folding*, *in* HIGH PERFORMANCE COMPUTING SYS. & APPLICATIONS 333, 334 (Jonathan Schaeffer ed., 1998) (describing the use of computational methods to minimize known thermodynamic potential of an astronomical number of potential structures with each amino-acid unit able to adopt several distinct conformations by function minimization using genetic algorithms).

11. Ryan L. Marson, Trung Dac Nguyen & Sharon C. Glotzer, *Rational Design of Nanomaterials from Assembly and Reconfigurability of Polymer-Tethered Nanoparticles*, 5 MATERIALS RES. SOC'Y COMM. 397, 397–98 (2015) (explaining that the rational design of nanomaterials via computer simulation identifies target nanostructures, candidate-building blocks, and efficient assembly pathways, resulting in next generation materials that can self-assemble into complex, functional, and reconfigurable structures).

12. Throughout this Article, the term "chemical" also includes biochemical and materials science. Moreover, this Article's focus on chemical applications refers to any unpredictable art areas where computational experimentation could be utilized by an inventor.

13. *See* U.S. PATENT & TRADEMARK OFFICE, MANUAL OF PATENT EXAMINING PROCEDURE § 2164.02 (9th ed. 2018) [hereinafter MPEP], https://mpep.uspto.gov/RDMS/MPEP/current#/current/d0e18.html [https://perma.cc/CPF6-PYGY] (noting that an example in a U.S. patent application may be "prophetic" and describe an embodiment of the invention based on predicted results rather than work actually conducted or results actually achieved); Lemley, *supra* note 4, at 1179 (explaining that courts have permitted an applicant to use "prophetic examples," which are guesses as to what would happen if the inventor were to build and test the invention).

14. *See* Atlas Powder Co. v. E.I. du Pont de Nemours & Co., 750 F.2d 1569, 1577 (Fed. Cir. 1984); Bratislav Stanković, *The Use of Examples in Patent Applications*, 18 INTELL. PROP. & TECH. L.J. 9, 10 (2006) (stating that US patent law allows for the use of prophetic examples and for simulated or predicted test results of properties).

computational experiments to predict chemical functions, properties, reactions, and structures with high accuracy and thereby gain quicker issuance of the patent application. The result would be that the researcher-inventor would gain market exclusivity by preventing others from making, using, selling, or offering to sell[15] an entire class of chemical compounds.

While advancements in computational research enable inventors to test hypotheses more easily and quickly, computational capabilities also challenge US patent law doctrines. In part, computational research has made experimentation a "hunting license."[16] As examples, molecular dynamics simulations and both machine learning and deep learning enable inventors to describe hypothetical chemical structures and their properties in the specification of a patent application, develop prophetic examples,[17] and file patent claims of a broad genus[18] without necessarily providing adequate support. Computational technology allows inventors to give an appearance of reduction to practice[19] that may not have been performed yet. While computational capabilities advance and their adoption continues to proliferate among researchers, US patent law doctrines continue to assume that experimentation is only a traditional laboratory exercise. For example, the enablement determination, which relies on the *Wands* factors[20] to assess the degree of undue experimentation, does not consider computational-specific experimentation. As an additional example, the utility determination is unclear on evaluation of hypothetical chemical structures.[21] This Article suggests that advancements in computation have outpaced

15. 35 U.S.C. § 271(a) (2018) ("Except as otherwise provided in this title, whoever without authority makes, uses, offers to sell, or sells any patented invention, within the United States or imports into the United States any patented invention during the term of the patent therefor, infringes the patent.").

16. *See* Brenner v. Manson, 383 U.S. 519, 536 (1966) ("But a patent is not a hunting license. It is not a reward for the search, but compensation for its successful conclusion.").

17. MPEP, *supra* note 13, § 2164.02 ("An example may be 'working' or 'prophetic.' A working example is based on work actually performed. A prophetic example describes an embodiment of the invention based on predicted results rather than work actually conducted or results actually achieved.").

18. *Id.* § 806.04 (suggesting that a genus is defined as a generic invention, such that it claims more than one patentably distinct species; explaining that in US patent prosecution practice, a patent examiner may require the applicant in a reply to a US Office action to elect a species of the invention to which the patent claim will be restricted if no claim to the genus is found to be allowable).

19. *See id.* § 2138.05(IV) (stating that reduction practice, which may be an actual reduction or a constructive reduction to practice, requires recognition and appreciation of the invention).

20. *See In re* Wands, 858 F.2d 731, 737 (Fed. Cir. 1988).

21. *In re* Fisher, 421 F.2d 1365, 1378 (Fed. Cir. 2005).

determinations in major patent cases, and these advancements have conflated key patentability doctrines. The result of computational capabilities is that enablement becomes subsumed into the utility doctrine.

The benefit of advancements in computational research capabilities for inventors is not in question. Inventors are allowed to use computational tools to aid in conception and reduction to practice. Instead, the discussion should center around the disruption, potential response, and patent policy implications of US patent law doctrines caused by the advent and proliferation of computational research capabilities in science and engineering research of chemical compounds and structures. The key questions that are at the heart of this Article are as follows: (1) What are the doctrinal patent law implications that follow from advancements in computational experimentation?; (2) How should patent examination at the United States Patent & Trademark Office (USPTO) be reformed in light of inventors' use of computational tools for experimentation?; and (3) What are the patent policy considerations for computational experimentation as it stands now and in response to proposed reforms suggested herein?

Few scholars have addressed experimentation in US patent law and in such cases, have written minimally and in a disapproving tone of prophetic examples.[22] To date, no legal scholarship has addressed computational research capabilities and their impact on patent law doctrine and policy. One article studied patent law disclosure doctrines through the Norden model.[23] Another article empirically analyzed prophetic examples to determine harms with abandonment rates of patents and misleading scientists, proposing that prophetic examples should be conceptualized as hypotheses rather than prophecies.[24]

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22. *See* Timothy R. Holbrook, *Possession in Patent Law*, 59 S.M.U. L. REV. 123, 158 (2006) ("[P]rophetic examples cannot allow the patent claim to extend beyond what the inventor possessed."); Lemley, *supra* note 4, at 1179 ("If that guess [of a prophetic example] turns out to be reasonably accurate, the paper patentee gets credit for teaching others how to make and use the invention even though she never did so herself."); Lisa Larrimore Ouellette, Pierson, *Peer Review, and Patent Law*, 69 VAND. L. REV. 1825, 1830 (2016) (describing an anecdote where "'prophetic examples' written to support a 'constructive reduction to practice' rather than actual results from a working device [in order to illustrate] the frequent award of patents earlier than is socially optimal"); Seymore, *Heightened Enablement*, *supra* note 1, at 145 ("[A] patent supported with prophetic examples poses the danger of rewarding an inventor with undue patent scope.").

23. Greg R. Vetter, *Patent Law's Unpredictability Doctrine and the Software Arts*, 76 MO. L. REV. 764, 764, 769 (2011) (suggesting that the Norden Model, a staple in cost and staff estimating studies, "helps illustrate the doctrinal potency of undue experimentation and unpredictability in terms of effort for a follow-on artisan attempting to make and use the invention based on the patent disclosure"; arguing that the unpredictable technology doctrine should not be applied categorically, but rather should be a more flexible, fine-grained approach).

24. Janet Freilich, Prophetic Patents 1, 50, 59 (June 25, 2018) (unpublished manuscript), https://papers.ssrn.com/sol3/papers.cfm?abstract_id=3202493 [https://perma.cc/K4Q4-KD4T]

Unlike prior scholarship that has critiqued and empirically evaluated prophetic examples, this Article focuses on technological foundations, doctrinal disruptions and applications, ways of rethinking doctrines, and reform and policy considerations of computational experimentation advancement and proliferation in the unpredictable arts. It focuses on the doctrinal challenges to the enablement and utility requirements of patentability in US patent law in light of advancements in computational experimentation capabilities that are displacing or complementing traditional, laboratory-based synthetic chemistry experiments.

This Article's purpose is not to replay an empirical and historical analysis of prophetic examples. Rather, the purpose is to present computationally derived inventions in a new light through multiple avenues, including: an explanation of the technological causes,[25] an illumination of doctrinal challenges,[26] applications of doctrinal disruptions, a normative claim about enablement and utility,[27] a proposal for reforming patentability and patent examination, and a discussion of implications for innovation policy.[28] This Article is the first academic paper to connect molecular dynamics simulations, as well as machine learning and deep learning technologies, to patent law doctrines in order to explain doctrinal patent law disruptions caused by such emerging technologies. In doing so, it fills a gap in patent law scholarship and contributes to ongoing debates concerning optimal patent filing timing, incentives for inventors' actual and constructive reduction to practice, and institutional patent examination procedures. It is part of a larger research initiative that analyzes how patent law influences and is influenced by emerging digital technologies and bridges patent law with data science, computation, and artificial intelligence. This Article also serves as a guide to science and engineering researcher-inventors, as well as patent attorneys who represent them, technology transfer professionals, and in-house patent counsel involved with research and development of chemical compounds, structures, and processes.

The Article proceeds as follows: Part II explores the transition from traditional laboratory research to computational research. It further explains how computational capabilities can enable *in silico*

(providing historical, theoretical, and empirical analysis of prophetic examples based on analysis of a novel dataset of over 2 million US patents and applications in biology and chemistry, and arguing for a shift from prophesies to more clearly delimited hypotheses).

25. *See infra* Part II.

26. *See infra* Part III.

27. *See infra* Part IV.

28. *See infra* Section V.C.

inventions by either complementing or displacing traditional laboratory research. Part III introduces the conceptual foundations of enablement, written description, and utility doctrines in US patent law. The review in Part III establishes the contours of the applicability of computational experimentation in US patent law in Part IV. It also illustrates the doctrinal tensions that emerge with computational experimentation and existing patent law frameworks and suggests that enablement becomes subsumed in utility for computationally derived inventions. Furthermore, Part IV brings insights from computational capabilities to present applications and demonstrates challenges to utility and enablement doctrines in US patent law. Part V provides reform proposals of a laboratory-based working example for the utility requirement and new computationally based hiring characteristics and training guidance for patent examination. It also responds to potential critiques of the reform proposals and discusses innovation policy underlying the proposed reforms. Part VI briefly concludes.

II. THE RISE OF COMPUTATIONAL RESEARCH

Experimentation is a core facet of scientific and engineering research, and allows for testing hypotheses and theories.[29] Classical, traditional experimental research in chemistry involves empirical observations and chemical alterations of substances occurring naturally in the environment through chemical synthesis.[30] During traditional laboratory experiments, researchers also vary parameters such as through design of experiments, in advance of synthesis to improve yields or to provide greater understanding of the factors underpinning a reaction.[31] However, such traditional methods are slow, time consuming, costly, and could involve utilizing expensive reagents, multiple steps, laboratory personnel, and equipment.[32]

Given these challenges, there has been a need to speed up, make cheaper, and improve success in biochemical, chemical, and materials

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29. *See* Schering Corp. v. Gilbert, 153 F.2d 428, 433 (2d Cir. 1946) (characterizing experimental science as having results that are uncertain, unpredictable, and unexpected).

30. *See* Vu, Quyen & Huong, *supra* note 6, at 61 ("In the distant past, designing a new drug by changing the molecular structure of an existing drug was a slow process of trial and error. . . . [Computational experimentation] can also identify those chemicals that would probably not be successful in treating a particular disease before time and money are invested in extensive testing.").

31. Paul M. Murray et al., *The Application of Design of Experiments (DoE) Reaction Optimisation and Solvent Selection in the Development of New Synthetic Chemistry*, 14 ORGANIC & BIOMOLECULAR CHEMISTRY 2373, 2374–75 (2016).

32. *Id.*; LAM ACTION, WHY IS SCIENTIFIC RESEARCH SO EXPENSIVE? (2015), http://lamaction.org/wp-content/uploads/2015/06/Scientific-research-expenses-explained.pdf [https://perma.cc/TJ56-S4HC].

science research. The rapid improvements in computer hardware and processing power have garnered the attention of science and engineering researchers who have introduced computational techniques to the forefront of traditional laboratory research. Thus, there has been a shift in traditional laboratory-based research towards information-focused research, for which computational research tools play a central research role.[33] Computational research is gaining traction in scientific and engineering research communities,[34] and it is either supplementing[35] or displacing traditional laboratory research.[36]

Research in science and engineering is being transformed by the development of new computational research tools. Namely, these tools advance exploration of the world and are the new paradigm for *in silico* exploration of otherwise inaccessible phenomena.[37] The increase in power of both computing hardware[38] and numerical algorithms[39] have made computational science critical to the US industrial economy and

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33. Michael S. Mahoney, *The History of Computing in the History of Technology*, 10 IEEE ANN. HIST. COMPUT. 113, 113 (1988).

34. Matt Shipman, *Why, and How, Computational Research Is Changing Materials Science*, N.C. ST. U. (Apr. 30, 2015), https://news.ncsu.edu/2015/04/mse-comp-research/ [https://perma.cc/P2BF-Z7GM] ("[W]e can now use models to design new materials that have a specific set of characteristics for use in any given application . . . . It would take years to evaluate those [material] combinations using traditional experimental methods, but we can narrow it down to a handful of the most promising materials combinations.").

35. Esteban P. Busso, *Multiscale Approaches: From the Nanomechanics to the Micromechanics*, *in* 514 CISM COURSES AND LECTURES: COMPUTATIONAL AND EXPERIMENTAL MECHANICS OF ADVANCED MATERIALS 141, 141 (Vadim V. Silberschmidt ed., 2010); Theresa Sperger, Italo A. Sanhueza & Franziska Schoenebeck, *Computation and Experiment: A Powerful Combination to Understand and Predict Reactivities*, 49 ACCT. CHEMICAL RES. 1311, 1312 (2016).

36. G. Wayne Brodland, *How Computational Models Can Help Unlock Biological Systems*, 47–48 SEMINARS CELL & DEVELOPMENTAL BIOLOGY 62, 65 (2015); Sanjay Chandrasekharan, Nancy J. Nersessian & Vrishali Subramanian, *Computational Modeling: Is This the End of Thought Experiments in Science?*, *in* THOUGHT EXPERIMENTS IN PHILOSOPHY, SCIENCE, AND THE ARTS 239, 239 (Mélanie Frappier et al. eds., 2013); Timothy Gould, *Welcome to Lab 2.0 Where Computers Replace Experimental Science*, CONVERSATION (July 24, 2016, 11:34 PM), https://theconversation.com/welcome-to-lab-2-0-where-computers-replace-experimental-science-57271 [https://perma.cc/UA55-MYC5].

37. Nicola Lettieri et al., *Ex Machina: Analytical Platforms, Law and the Challenges of Computational Legal Science*, 10 FUTURE INTERNET 37, 37–39 (2018) (suggesting that there are four paradigms of science, including (1) experimental science of describing phenomena, (2) theoretical science of modeling and generalization, (3) computational science of simulation of complex phenomena, and (4) exploratory science that is data intensive and involves statistical exploration with data mining; concluding that scientific computing plays a central role in research and that computational methods are now a standard part of the scientific practice).

38. John D. Owens et al., *GPU Computing*, 96 PROC. IEEE 879, 896 (2008); J. Tan & X. Fu, *Addressing Hardware Reliability Challenges in General-Purpose GPUs*, *in* ADVANCES IN GPU RESEARCH AND PRACTICE 649, 649 (Hamid Sarbazi-Azad ed., 2017).

39. JUSTIN SOLOMON, NUMERICAL ALGORITHMS, at xv (2015); Jerome H. Friedman, *Recent Advancements in Predictive (Machine) Learning*, 23 J. CLASSIFICATION 175, 181 (2006); Gelan Yang et al., *Recent Advancements in Signal Processing and Machine Learning*, 2014 MATHEMATICAL PROBS. ENGINEERING 1, 1 (2014).

central to research as a bridge between theory and experiments.[40] Increases in computing speed and capacity, as well as the availability of software packages, allow researchers to conduct computational experiments concerning reactivity, kinetics, and evolution of transition states in fields as diverse as materials science and biochemistry.[41] Some examples of recent advancements in computational techniques that permit computation experimentation are molecular dynamics simulations and both machine learning and deep learning technologies.

A. Molecular Dynamics Simulations

Experiments of the molecular level are no longer restricted to the laboratory and can be conducted computationally. Advancements in computing power are enabling simulations and predictions of biochemical properties and material properties with high precision.[42] As a result of Moore's Law doubling computing power every twenty-four months,[43] molecular dynamics simulations have developed to enable calculation of materials' properties.[44] The availability of more computational resources allows for molecular dynamics simulations of thousands of atoms over nanosecond timescales.[45]

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40. STEERING COMM. ON COMPUTATIONAL PHYSICS, COMPUTATION AS A TOOL FOR DISCOVERY IN PHYSICS: A REPORT TO THE NATIONAL SCIENCE FOUNDATION BY THE STEERING COMMITTEE ON COMPUTATIONAL PHYSICS 4, 9 (2017), https://www.nsf.gov/pubs/2002/nsf02176/nsf02176.pdf [https://perma.cc/CCC4-5DKL] (pointing out that much of the US industrial economy is based on material properties, like metals, plastics, semiconductors, and chemicals, so the potential economic impact of new materials' properties is huge, and an understanding of microscopic systems is central to many areas of science and engineering).

41. Wenfa Ng, What Drives Computation Chemistry Forward: Theory or Computer Power? 1 (Aug. 17, 2016) (unpublished manuscript), https://peerj.com/preprints/552/ [https://perma.cc/FS9V-95J3] ("Specifically, availability of large amount of computing power at declining cost, and advent of graphics processing unit (GPU) powered parallel computing are enabling tools for solving up to now intractable problems.").

42. *See* Jens Glaser et al., *Strong Scaling of General-Purpose Molecular Dynamics Simulations on GPUs*, 192 COMPUTER PHYSICS COMM. 97, 97–98 (2015) (describing the use of graphics processing units to accelerate investigation of thermodynamic properties).

43. MOORE'S LAW, http://www.mooreslaw.org/ [https://perma.cc/KEB9-XXE6] (last visited Feb. 5, 2019).

44. Peter Steneteg, *Development of Molecular Dynamics Methodology for Simulations of Hard Materials*, LINKÖPING U. INST. TECH. 1, 5 (2012), https://pdfs.semanticscholar.org/3965/7426f57a4b7fce24dfdd059708b3af0ed3eb.pdf [https://perma.cc/9UPZ-LB42] (describing the calculations of properties for paramagnetic materials based on atoms' "positions, velocities, and masses [in a] deterministic way to simulate the movement of the atoms" in femtosecond time steps).

45. *See* Jarosaw Meller, *Molecular Dynamics*, ENCYCLOPEDIA LIFE SCI. 1, 4, 7–8 (2001), https://dasher.wustl.edu/chem478/reading/md-intro-1.pdf [https://perma.cc/VVH7-64M5] (describing numerically solving quantum and statistical equations of atoms to identify diffusion pathways, ligand-protein interactions, interatomic potentials, substrate-inhibitor binding to proteins for the design of vaccines, drugs, peptides, and small proteins).

Molecular dynamics simulations enable researchers to understand properties of molecules either before conducting traditional laboratory experiments or in conjunction with synthesis. Such simulations provide predictions about interactions between molecules, which enable predictions of bulk properties.[46] These techniques can provide quantitative predictions of molecular structures, interactions, and functionality for virtual, high throughput screening and drug design.[47]

B. Machine Learning and Deep Learning Technologies

Machine learning is simply a form of data analysis that uses algorithms to continuously learn from data by recognizing hidden patterns without being programmed to do so.[48] Molecular dynamics simulations are based on reproducing molecular scale chemistry and physics. In contrast, both machine learning[49] and deep learning[50] techniques produce useful models[51] that can predict chemical and biological properties of compounds.[52] Even traditional chemical

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46. Michael P. Allen, *Introduction to Molecular Dynamics Simulation*, 23 COMPUTATIONAL SOFT MATTER: FROM SYNTHETIC POLYMERS TO PROTEINS 1, 1 (describing that molecular dynamics simulations provide properties of "transport coefficients, time-dependent responses to perturbations, rheological properties[,] and spectra").

47. Maithri Gundaram et al., *Computational Drug Design and Molecular Dynamic Studies – A Review*, 6 INT'L J. BIOMEDICAL DATA MINING 1, 3, 5 (2016) (describing the use of molecular dynamics simulations for identifying potent drug molecules).

48. TOM M. MITCHELL, MACHINE LEARNING 1 (Eric M. Munson ed., 1997), https://www.cs.ubbcluj.ro/~gabis/ml/ml-books/McGrawHill%20-%20Machine%20Learning%20-Tom%20Mitchell.pdf [https://perma.cc/JC4G-FMJW].

49. Yann LeCun, Yoshua Bengio & Geoffrey Hinton, *Deep Learning*, 521 NATURE 436, 436 (2015) (comparing machine learning with deep learning, a sub-set of machine learning, and specifying that machine learning techniques "were limited in their ability to process natural data in their raw form"). Machine learning is restricted to internal representations from which the learning subsystem can detect or classify patterns in the input. *Id.* By contrast, however, deep-learning is an advancement of machine learning, providing multiple levels of representation such that very complex functions can be learned. *Id.* Unlike machine learning, the key aspect of deep learning is that layers of features are not designed by human engineers but are "learned from data using a general-purpose learning procedure." *Id.*

50. Garrett B. Goh, Nathan O. Hodas & Abhinav Vishnu, *Deep Learning for Computational Chemistry*, 16 J. COMPUTATIONAL CHEMISTRY 1291, 1295 (2017); *id.* at 1291 (providing as examples, the Merck Activity Prediction Challenge in 2012, where a deep learning network outperformed Merck's internal baseline model without a single chemist or biologist, and the NIH's Tox21 toxicity prediction challenge, which predicted activity and toxicity for a number of chemical compounds).

51. Kristof T. Schütt et al., *Quantum-Chemical Inisghts from Deep Tensor Neural Networks*, 8 NATURE COMM. 13890, at 1 (2018) (providing a model of classification of aromatic rings with respect to their stability, based on a deep learning approach that enables spatially and chemically resolved insights into quantum-mechanical properties of molecular systems).

52. John B. O. Mitchell, *Machine Learning Methods in Chemoinformatics*, 4 WIREs COMPUTATIONAL MOLECULAR SCI. 468, 468 (2014) (explaining that machine learning can predict bioactivity, toxicological, pharmacological, and physiochemical properties).

synthesis techniques combined with optimization techniques are tedious, time consuming, based on trial and error, and labor intensive; however, machine learning provides for simulation of chemical properties and reaction pathway identification that transform chemical ideas into reality more quickly and accurately.

Such computational techniques accelerate drug discovery,[53] genomics,[54] and materials design.[55] Machine learning can be used in chemistry to construct structure-activity relationships, predict properties of molecules, predict chemical reactions,[56] and discover hidden information in chemicals.[57] Machine learning has been and continues to be applied in biomedical and chemical settings, such as process optimization in chemical manufacturing, drug design in medicinal chemistry, toxicity prediction, and chemical compound classification.[58] Such techniques are also being applied in materials science for macroscopic and microscopic materials performance prediction for discovery of new materials.[59] These examples highlight

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53. Hongming Chen et al., *The Rise of Deep Learning in Drug Discovery*, 23 DRUG DISCOVERY TODAY 1241, 1241–42 (2018); Jon Paul Janet, Lydia Chan & Heather J. Kulik, *Accelerating Chemical Discovery with Machine Learning: Simulated Evolution of Spin Crossover Complexes with an Artificial Neural Network*, 9 J. PHYSICAL CHEMISTRY LETTERS 1064, 1064–71 (2018); Antonion Lavecchia, *Machine-Learning Approaches in Drug Discovery: Methods and Applications*, 20 DRUG DISCOVERY TODAY 318, 318 (2015).

54. Maxwell W. Libbrecht & William Stafford Noble, *Machine Learning Applications in Genetics and Genomics*, 16 NATURE REV. GENETICS 321, 321–32 (2015); Tianwei Yue & Haohan Wang, *Deep Learning for Genomics: A Concise Overview* 1, 2 (ArXiv, Working Paper No. 1802.00810, 2018), https://arxiv.org/abs/1802.00810 [https://perma.cc/4TNZ-SDQJ].

55. Tim Mueller, Aaron Gilad Kusne & Rampi Ramprasad, *Machine Learning in Materials Science: Recent Progress and Emerging Applications*, *in* 29 REVIEWS IN COMPUTATIONAL CHEMISTRY 186, 186 (Abby L. Parrill & Kenny B. Lipkowitz eds., 2016) (describing how to predict properties using quantum-derived data and machine learning to identify "atomization energy, the formation energy, the lattice constant, the spring constant, the band gap, the electron affinity, and the optical and static components of the dielectric constant").

56. Matthew A. Kayala et al., *Learning to Predict Chemical Reactions*, 51 J. CHEMICAL INFO. & MODELING 2209, 2211 (2011) (explaining a new chemical reaction framework where mechanistic reactions are modeled as interactions); Zhenpeng Zhou, Xiaocheng Li & Richard N. Zare, *Optimizing Chemical Reactions with Deep Reinforcement Learning*, 3 ACS CENT. SCI. 1337, 1337 (2017) (describing the use of a new Deep Reaction Optimizer model to guide interactive decision-making procedure in optimizing reactions by finding the optimal reaction condition with the least number of steps).

57. Vorgelget Von, Novel Machine Learning Methods for Computational Chemistry 2–3 (June 19, 2012) (unpublished dissertation, Berlin Institute of Technology) (summarizing that machine learning can be utilized for drug discovery to predict properties of absorption, distribution, metabolism, excretion, and toxicity, or ADMET, and physiochemical properties of small molecules in place of the traditional experimental side of research; suggesting that machine learning technologies can be applied for drug discovery for virtual screening of compounds with respect to different properties).

58. Matthew N.O. Sadiku, Sarhan M. Musa & Osama M. Musa, *Machine Learning in Chemical Industry*, 3 INT'L. J. ADVANCES SCI. RESEARCH & ENGINEERING 12, 13 (2017).

59. Yue Liu et al., *Materials Discovery and Design Using Machine Learning*, 3 J. MATERIOMICS 159, 164 (2017) ("[P]roperties of materials, such as hardness, melting point, ionic

the increasing use of computational experimentation and support the need for it to be addressed by patent law doctrines.

III. DOCTRINAL US PATENT LAW FOUNDATIONS

The rapid proliferation of computation in sciences and engineering research raises doctrinal patent law challenges. The use of molecular dynamics simulation[60] and both machine learning and deep learning technologies requires discussion and reconsideration of the unpredictable arts in US patent law. The doctrinal disruptions identified herein do not apply to the predictable arts, but rather are unique to the unpredictable arts, which are characterized by requiring experimentation.[61]

The predictable arts refer to applied technologies of electrical engineering and mechanical engineering in US patent law and are rooted in well-defined and predictable factors.[62] Artisans of applied technologies can utilize mathematics and physics principles to predict properties, construct alternate embodiments, and foresee performance without difficulty. For example, mechanical engineers can use mechanical properties of materials to calculate pipeline flexure stresses[63] or use principles of thermodynamics and heat transfer to design heat exchangers, internal-combustion engines, and gas turbines.[64] Also, once one embodiment of an invention in the predictable arts is described (i.e., one heat exchanger), artisans can easily predict how other embodiments within the claimed scope can be made and used (i.e., dimensions and geometry of varying kinds of heat exchangers).[65]

Unlike predictable arts, unpredictable arts are not well-defined. In unpredictable arts, small changes in the structure of an invention can yield vastly different properties and functions.[66] For example, in

conductivity, glass transition temperature, molecular atomization energy, and lattice constant, can be described at either the macroscopic or microscopic level [with machine learning techniques].").

60. *See supra* Section II.A.

61. Schering Corp. v. Gilbert, 153 F.2d 428, 433 (2d Cir. 1946) (characterizing experimental science as having results that are uncertain, unpredictable, and unexpected).

62. *In re* Vaeck, 947 F.2d 488, 496 (Fed. Cir. 1991) (noting that there is less necessary disclosure for predictable electrical or mechanical elements than unpredictable ones).

63. EUGENE A. AVALLONE & THEODORE BAUMEISTER III, MARKS' STANDARD HANDBOOK FOR MECHANICAL ENGINEERS ch. 5, at 1–55 (10th ed. 1996) (explaining strength of materials).

64. *Id.* ch. 9, at 75–133.

65. David Tseng, *Not All Patents Are Created Equal: Bias Against Predictable Arts Patents in the Post-KSR Landscape*, 13 CHI.-KENT J. INTELL. PROP. 165, 167 (2013).

66. Sean B. Seymore, *Rethinking Novelty in Patent Law*, 60 DUKE L.J. 919, 935 (2011) [hereinafter Seymore, *Rethinking Novelty*].

biotechnology, chemistry, and nanotechnology, a minor alteration in a functional chemical compound may render it inert or make it highly reactive.[67] As such, US patent law requires that specifications concerning unpredictable arts contain more detail than those of predictable arts.[68] Thus, the more unpredictable a field of art and the more uncertain or unexpected the result, the more disclosure is required to enable a patent claim.[69] Therefore, unpredictable technologies require inventors to provide more examples, experimental results, and tables[70] so that a person having ordinary skill in the art (PHOSITA) can carry out the steps necessary to produce a similar compound with similar properties and functions.[71]

A challenge with the unpredictable arts arises with enablement—a patentability lever requiring that a PHOSITA be able to make and use an invention without undue experimentation.[72] The enablement patentability requirement is challenging to assess for unpredictable technologies because a PHOSITA cannot easily predict the reactivity or outcomes.[73] It may be challenging to assess if examples provided in the specification are sufficient to make or use an invention in the unpredictable arts if the patent claim scope is too broad. For example, in *Pharmaceutical Resources, Inc. v. Roxane Laboratories*, the United States Court of Appeals for the Federal Circuit addressed enablement with broad patent claims encompassing hundreds of possible surfactants of a highly unpredictable chemical structure.[74] The Federal Circuit rejected an argument that a hypothetical pharmaceutical formulator could start experimenting with surfactants to practice the invention, and held that limited working examples did not provide enablement commensurate with the patent claim scope.[75] Thus, *Pharmaceutical Resources* demonstrates that the degree of

67. *See, e.g.*, *id.* at 935.

68. *In re* Fisher, 427 F.2d 833, 840 (C.C.P.A. 1970) ("In cases involving unpredictable factors, such as most chemical reactions and physiological activity, the scope of enablement obviously varies inversely with the degree of unpredictability. . . .").

69. Spectra-Physics, Inc. v. Coherent, Inc., 827 F.2d 1524, 1533 (Fed. Cir. 1987) ("If an invention pertains to an art where the results are predictable, . . . a broad claim can be enabled by disclosure of a single embodiment.").

70. *See* Stanković, *supra* note 14, at 10.

71. *See* Seymore, *Heightened Enablement*, *supra* note 1, at 137.

72. Sean B. Seymore, *The Enablement Pendulum Swings Back*, 6 NW. J. TECH. & INTELL. PROP. 278, 279 (2008) [hereinafter Seymore, *Enablement Pendulum*].

73. Sean B. Seymore, *Foresight Bias in Patent Law*, 90 NOTRE DAME L. REV. 1105, 1115 (2015) [hereinafter Seymore, *Foresight Bias*].

74. Pharm. Res., Inc. v. Roxane Labs., Inc., 253 F. App'x. 26, 29–30 (Fed. Cir. 2007) (reasoning that a large part of the asserted patent claims' scope was directed to inoperative embodiments and combinations and that the three working examples did not provide enabling disclosure that was commensurate with the claims' scope).

75. *Id.* at 30–31.

experimentation to make or use the invention as patent claims through examples in the specification is challenging in the unpredictable arts.

The advent and proliferation of computational technologies in the research and development of the unpredictable arts complicates the enablement requirement further. This is because these inventions generate data distinct from the operation and use of the invention.[76] The data generated by computational research tools can be utilized to describe hypothetical composition of matter structures, as well as hypothetical processes in the patent specification and prophetic examples. While computational research tools enable an inventor to craft a patent specification or patent claims that can be considered hypothetical or prophetic, the words in the patent specification may not meet enablement.

Another challenge with the unpredictable arts arises with utility, which is rarely a difficult hurdle[77] except in some of the unpredictable arts where results are often uncertain and uncovered through experimentation.[78] The utility patentability requirement is challenging to assess for unpredictable technologies since they are pioneering and their effectiveness has not yet been established.[79] Computational design in unpredictable fields potentially makes utility a more challenging threshold since chemical intermediates might be computationally designed to have desirable properties, and therefore, difficult to assess under the current standard.[80]

The advent of computational experimentation creates doctrinal challenges with enablement and utility doctrines that are associated with prophesizing early results,[81] patent examination,[82] and the

76. Brenda M. Simon & Ted Sichelman, *Data-Generating Patents*, 111 NW. L. REV. 377, 379 (2017) (explaining that so-called data-generating inventions, which are defined as invention that generate unique data from users, can generate large amounts of data about the world in general, and in doing so, improve the operation of the invention).

77. Michael Risch, *A Surprising Useful Requirement*, 19 GEO. MASON L. REV. 57, 58 (2011) (noting that inventions which fail to meet the current utility patentability standard are rare).

78. *See* Seymore, *Serendipity*, *supra* note 5, at 190 (considering that accidents may become inventions, and in some cases conducting experiments will help reduce the conceived idea to practice).

79. Michael Risch, *Reinventing Usefulness*, BYU L. REV. 1195, 1198–99, 1202 (2010) (suggesting that prophetic inventions, which are more common in unpredictable arts, could work but would be viewed as unworkable even by someone familiar with the subject matter).

80. Sean B. Seymore, *Making Patents Useful*, 98 MINN. L. REV. 1046, 1079 (2014) [hereinafter Seymore, *Making Patents Useful*] (suggesting that inventors can concoct trivial uses simply to satisfy the utility requirement, but chemical intermediates may not be patentable as such).

81. *See* Freilich, *supra* note 24, at 42.

82. *See infra* Section V.B.

presumption of patentability.[83] Computational technologies make the speculation-experimentation balance a challenge in multiple ways. First, inventors may attempt to utilize computational tools to claim broadly, even though they know of only a small number of working examples.[84] Second, computational tools make it easier to develop prophetic examples[85] and file earlier patent applications, such that inventors may file patent applications prior to proving out the technology.[86] Third, inventors may use computational tools to formulate small changes to a chemical structure and attempt to claim broader properties than the inventive concept.[87] In sum, computational tools can enable an inventor to make a patent application appear as if experimental data has been achieved when, in fact, there have been only computational simulations of hypothetical experiments, thus resulting in prophetic examples. These doctrinal problems caused by computational experimentation are explained and applied to examples in detail in Part IV of this Article.

A. Enablement and Undue Experimentation

US patent law embraces a contract metaphor in the sense that disclosure is the price for the limited exclusivity provided for the invention.[88] The disclosure is the quid pro quo of the right to exclude as required by patent law and is governed by 35 U.S.C. § 112(a), which requires the following:

> The specification shall contain a written description of the invention, and of the manner and process of making and using it, in such full, clear, concise, and exact terms as to enable any person skilled in the art to which it pertains, or with which it is most nearly connected, to make and use the same, and shall set forth the best mode contemplated by the inventor or joint inventor of carrying out the invention.[89]

Thus, under section 112(a) of the Patent Act, an inventor has an obligation to disclose a written description and provide enablement (i.e., how to make and use the invention). There are strategic and economic reasons why an inventor may not disclose the invention

83. Sean B. Seymore, *The Presumption of Patentability*, 97 MINN. L. REV. 990, 995 (2013) [hereinafter Seymore, *The Presumption of Patentability*] (explaining that a patent application enjoys the presumption of patentability at the time of filing the patent application).

84. *See supra* Section IV.A.2.

85. *See* MPEP, *supra* note 13, § 2164.02 ("A prophetic example describes an embodiment of the invention based on predicted result rather than work actually conducted or results actually achieved.").

86. *See* Freilich, *supra* note 24, at 17 (stating that applicants who choose prophetic examples can file a patent application earlier than those who run experiments).

87. *See supra* note 72 and accompanying text.

88. THOMAS G. FESSENDEN, AN ESSAY ON THE LAW OF PATENTS 48–49 (1st ed. 1810).

89. 35 U.S.C. § 112(a) (2018).

adequately in the patent application[90] or choose not to disclose the invention entirely and instead pursue trade secret protection.[91] The following Section explains two separate and distinct requirements of the specification in the patent instrument and how they relate to utility, another patentability requirement.

One of the main functions of the patent document is to provide full disclosure to the public about the invention in return for a limited period of exclusivity conferred by the patent.[92] Enablement is the patentability requirement that satisfies this teaching function of the patent. In order to meet enablement, the specification of the patent document must describe how to make and use the invention to a PHOSITA.[93] Courts have read the enablement requirement to require that the patentee disclose sufficient information, which is determined based on a number of factors:

(1) the quantity of experimentation necessary;
(2) the amount of direction or guidance provided;
(3) the presence or absence of working examples;
(4) the nature of the invention;
(5) the state of the prior art;

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90. In patent law practice, a patent attorney or a patent agent may provide suggest to an inventor numerous reasons why the inventor may not want to adequately disclose an invention, including (1) strategically disclosing sufficient information to garner satisfying the requirements of 35 U.S.C. § 112(a) and hoping for issuance of the patent, (2) conducting ongoing constructive reduction to practice, but having advanced the invention enough to warrant filing a patent application for actual reduction to practice, and/or (3) filing what would be parent patent application from which to file subsequent patent applications as continuing-in-part (CIP) patent applications, from which there would be more disclosure and with a later file date. Adequate disclosure is an important consideration for nascent technologies in the biotechnology, chemical, and materials science fields, particularly for composition of matter patent claims, and is magnified by the advent and prevalence of computational capabilities in these scientific and technological fields of research. *See infra* Section IV. This Article focuses on how the phenomena of computational experimentation (as defined herein) affects and influences why an inventor may not disclose the invention adequately yet may still meet the 35 U.S.C. § 112(a) patentability requirement. Patent policy consideration for adequate disclosure include incentives to inventors, timing of disclosure compliance, and temporal paradox, and each of these issues discussed in this Article. *See infra* Section IV.A.

91. United States v. Dubilier Condenser Corp., 289 U.S. 178, 186 (1933) (recognizing that an inventor "may keep his invention secret and reap its fruits indefinitely," but that "[i]n consideration of its disclosure and the consequent benefit to the community, the patent is granted").

92. Pfaff v. Wells Elecs., Inc., 525 U.S. 55, 63 (1998) ("[T]he patent system represents a carefully crafted bargain that encourages both the creation and the public disclosure of new and useful advances in technology, in return for an exclusive monopoly for a limited period of time."); Bonito Boats, Inc. v. Thunder Craft Boats, Inc., 489 U.S. 141, 151 (1989) ("[T]he ultimate goal of the patent system is to bring new designs and technologies into the public domain through disclosure"); Kewanee Oil Co. v. Bicron Corp., 416 U.S. 470, 480–81 (1974) ("In return for the right of exclusion . . . the patent laws impose upon the inventor a requirement of disclosure.").

93. 35 U.S.C. § 112(a) (2018).

(6) the relative skill of those in the art;
(7) the predictability or unpredictability of the art; and
(8) the breadth of the claims.[94]

These factors determine whether a patent specification requires undue experimentation[95] to produce the claimed embodiments. These factors, known as the *Wands* factors, can be manipulated to modulate the enablement threshold.[96] Unpredictability, the seventh factor, is particularly important among the *Wands* factors and is broadly interpreted in the unpredictable arts.[97] While the assessment of the *Wands* factor for enablement is considered subjective,[98] it can be utilized to ferret out a truly impossible invention.[99] While the *Wands* factor assessment is the seminal test for enablement, there is not an explicit way to assess prophetic examples, which are seemingly omitted in their entirety.[100]

B. Written Description

The written description requirement is distinct but related to enablement. Both enablement and written description are disclosure obligations,[101] with enablement related to the teaching function of patent[102] and the written requirement related to possession of the invention.[103] The written description requirement necessitates that the applicant disclose a description of the invention to a PHOSITA in a way that demonstrates that the applicant possessed the invention at the time of filing his application.[104] In other words, the patentee must

94. See *In re* Wands, 858 F.2d 731, 737 (Fed. Cir. 1988).

95. *See id.*

96. Sean B. Seymore, *Uninformative Patents*, 55 HOUS. L. REV. 377, 386 (2017).

97. *See* Vetter, *supra* note 23, at 766, 800–01 (suggesting that the unpredictability of the *Wands* factors seem to operate categorically and, as a result, truncates the inquiry of the first *Wands* factor on experimentation and whether it is undue).

98. Alan L. Durham, *Patent Scope and Enablement in Rapidly Development Arts*, 94 N.C. L. REV. 1099, 1108 (2016) (noting that the assessment of the *Wands* factors is a matter of degree and is illustrative rather than mandatory).

99. Sean B. Seymore, *Patently Impossible*, 64 VAND. L. REV. 1491, 1532–34 (2017) (providing an example rejection of a patent application by an applicant who attempted to claim a method of using heat to transform antimony into gold, based on identifying a *Type I* impossibility through a working example).

100. *See* Freilich, *supra* note 24, at 17.

101. *See* Seymore, *Making Patents Useful*, *supra* note 80, at 1083–84.

102. *See* Sean B. Seymore, *Patenting the Unexplained*, 96 WASH. U. L. REV. (forthcoming 2019) (manuscript at 717), https://papers.ssrn.com/sol3/papers.cfm?abstract_id=3122761 [https://perma.cc/9L92-557V].

103. *See* Timothy R. Holbrook, *Patent Anticipation and Obviousness as Possession*, 65 EMORY L.J. 987, 990–91 (2016).

104. *See* Holbrook, *supra* note 22, at 127.

describe the invention in such a way "that one skilled in the art can clearly conclude that 'the inventor invented the claimed invention.'"[105]

The written description demonstrates that the inventor created and possessed the invention and serves as a public notice to communicate that the invention has been acquired by the inventor.[106] The purpose of the written description is to ensure that the applicant retained the invention disclosed in the originally filed application[107] and to show adequate support in the specification to show possession of the invention at the time of filing the patent application. The USPTO previously issued written description guidelines concerning the possession test,[108] and the Federal Circuit has stated that the specification must demonstrate possession of the invention.[109] Recently, the Federal Circuit stated that an inventor must possess the claimed invention on the filing date to meet the written description requirement.[110] However, possession by itself has been shown to be nebulous concept, and enablement has been proposed to be the best mechanism to show possession.[111] A recently filed petition for a writ of certiorari, which the Supreme Court denied, had alleged that the

105. Regents of Univ. of Cal. v. Eli Lilly & Co., 119 F.3d 1559, 1566 (Fed. Cir. 1997) (quoting Lockwood v. Am. Airlines, Inc., 107 F.3d 1565, 1572 (Fed. Cir. 1997)).

106. *See* Holbrook, *supra* note 22, at 127 (discussing that the test for the sufficiency of the written description of the invention is whether the patent demonstrates that that applicant was in possession of the full scope of the patent claims at the time that she filed her application).

107. *See* Durham, *supra* note 98, at 1105 (pointing out that Federal Circuit has used the written description requirement to invalidate patent claims that are broader than what the inventor "possessed" at the time of filing the patent application even if the claims did not change during the patent prosecution process).

108. *See* MPEP, *supra* note 13, § 2163 (restating the "possession" test and attempting to clarify its application by stating: "Whether the specification shows that applicant was in possession of the claimed invention is not a single, simple determination, but rather is a factual determination reached by considering a number of factors. Factors to be considered in determining whether there is sufficient evidence of possession include the level of skill and knowledge in the art, partial structure, physical and/or chemical properties, functional characteristics alone or coupled with a known or disclosed correlation between structure and function, and the method of making the claimed invention. Disclosure of any combination of such identifying characteristics that distinguish the claimed invention from other materials and would lead one of skill in the art to the conclusion that the applicant was in possession of the claimed species is sufficient.").

109. *See* Ariad Pharm., Inc. v. Eli Lilly & Co., 598 F.3d 1336, 1351 (Fed. Cir. 2010).

110. *See* Amgen Inc. v. Sanofi, 872 F.3d 1367, 1373 (Fed. Cir. 2017) (clarifying the written description as applied to antibodies and stating that "[t]o show invention, a patentee must convey in its disclosure that it 'has possession of the claimed subject matter as of the filing date.'"; nothing that possession "requires a precise definition" of the invention, where the "precise definition" requires the patentee to disclose "a representative number of species falling within the scope of the genus or structural features common to the members of the genus so that one of skill in the art can 'visualize or recognize' the members of the genus").

111. *See* Holbrook, *supra* note 22, at 146–47 (suggesting that possession refers to whether or not an inventor can make a functioning invention, and proposing that meeting enablement demonstrates possession).

Federal Circuit has reimagined the statutory standard by requiring possession of the claimed invention at the filing date. Accordingly, the petition urged the Court to take up the case to avoid deterring companies from innovation.[112]

C. Utility

Section 101 of the Patent Act mandates utility as a patentability requirement.[113] Utility seems to suggest an invention must be useful; yet, the statute does not clarify the meaning of "useful" and Congress has never defined the meaning of "useful" for US patent law. Remarks in early patent cases concerning utility suggested that inventions must have some beneficial use in society.[114] The utility requirement generally necessitates a minimal showing of the invention's pragmatic result,[115] but it is a more significant hurdle to patentability in the unpredictable arts.[116]

More complex and modern issues concerning utility began to arise with advancements in biotechnology, chemistry, and pharmaceuticals. In such applications, inventors were incentivized to obtain patent protection on compounds before laboratory testing and clinical trials. In doing so, inventors encountered obstacles with the utility requirement. The landmark utility case, *Brenner v. Manson*, addressed this situation. In *Brenner*, an inventor filed a patent application prior to synthesis of steroid compounds. The Supreme Court infamously stated that "a patent is not a hunting license [since] [i]t is not a reward for the search, but compensation for its successful conclusion."[117]

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112. Petition for Writ of Certiorari, Amgen v. Sanofi, 2019 WL 113092 (Jan. 7, 2019) (No. 18-127).

113. *See* 35 U.S.C. § 101 (2018) ("Whoever invents or discovers any new and *useful* process, machine, manufacture, or composition of matter . . . may obtain a patent." (emphasis added)).

114. *See* Lowell v. Lewis, 15 F. Cas. 1018, 1019 (C.C.D. Mass. 1817) (No. 8,568) ("All that the law requires is, that the invention should not be frivolous or injurious to the well-being, good policy, or sounds morals of society. The word "useful", therefore, is incorporated into the act in contradistinction to mischievous or immoral. . . . But if the invention steers wide of these objections, whether it be more or less useful is a circumstance very material to the interest of the patentee, but of no importance to the public. If it be not extensively useful, it will silently sink into contempt and disregard."); Bedford v. Hunt, 3 F. Cas. 37, 37 (C.C.D. Mass. 1817) (No. 1,217) ("[Patent law] does not look to the degree of utility; it simply requires that [the invention] shall be capable of use, and that the use is such as sound morals and policy do not discountenance or prohibit.").

115. Mitchell v. Tilghman, 86 U.S. 287, 397 (1873).

116. *See* Seymore, *Making Patents Useful*, *supra* note 80, at 1048–49.

117. Brenner v. Manson, 383 U.S. 519, 534–36 (1966) ("Until the process claim has been reduced to production of a product shown to be useful, the metes and bounds of that monopoly are not capable of precise delineation. . . . Such a patent may confer power to block whole areas of

The modern utility requirement in US patent law is comprised of the three prongs of credible utility, substantial utility, and specific utility.[118] Incredible utility—the negation of credible utility[119]—refers to wholly inoperative inventions,[120] such as a perpetual motion machine, cold fusion machine, or time machine. Therefore, credible utility is met with inventions that are operative and, in most cases, credible utility will be met. The concept of substantial and specific utility refers to practical utility,[121] which has been deemed interchangeable with "real world" utility.[122] Therefore, the substantial and specific utility requirement is met so long as the use is not so vague as to be meaningless and where the claimed invention has a significant and presently available benefit to the public.[123]

There is also a doctrinal connection between the utility requirement and the enablement requirement in US patent law.[124] In US patent law, if utility is not met, then enablement cannot be met either.[125] Plainly stated, one cannot describe how to make and use an invention if that invention is useless. As a result, arguments concerning the lack of usefulness of an invention are made both in the context of the utility requirement and the enablement requirement.[126] It is no surprise that utility rejections in the unpredictable arts are

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scientific development, without compensating benefit to the public. . . . A patent system must be related to the world of commerce rather than to the realm of philosophy.").

118. *See* Seymore, *Making Patents Useful*, *supra* note 80, at 1066–67 (discussing credible utility as referring to whether a PHOSITA would recognize an inventor's assertions as believable, substantial utility as referring to whether a PHOSITA would sue the invention to provide a significant and immediate benefit to the public, and specific utility as referring to whether an invention provide a well-defined and particular benefit to the public).

119. *See In re* Citron, 325 F.2d 248, 253 (C.C.P.A. 1963) (stating that utility was thought to be "incredible in light of the knowledge of the art, or factually misleading" when considered by the USPTO).

120. *See* MPEP, *supra* note 13, § 2107.01(II) (stating that an invention is "inoperative" when it does not operate to produce results claimed by the patent applicant).

121. *See id.* § 2107.01(I) ("Courts have used the labels 'practical utility,' 'substantial utility,' or 'specific utility' to refer to this aspect of the 'useful invention' requirement of 35 U.S.C. 101 . . . '[O]ne skilled in the art can use a claimed discovery in a manner which provides some immediate benefit to the public.'").

122. Nelson v. Bowler, 626 F.2d 853, 856 (C.C.P.A. 1980) (in which the applicant asserted that the composition was "useful" in a particular pharmaceutical application and provided evidence to support the assertion, and the court found that there was some immediate benefit to the public of the invention).

123. *See In re* Fisher, 421 F.3d 1365, 1371 (Fed. Cir. 2005) (clarifying that substantial and specific utility is not met when the claimed invention is not an end of the research effort but only a tool to be used along the way in search of practical utility).

124. *See* DONALD S. CHISUM, CHISUM ON PATENTS § 7.03(6) (2016).

125. *See* Process Control Corp. v. HydReclaim Corp., 190 F.3d 1350, 1358 (Fed. Cir. 1999) ("If a patent claim fails to meet the utility requirement because it is not useful or operative, then it also fails to meet the how-to-use aspect of the enablement requirement.").

126. *See In re* Brana, 51 F.3d 1560, 1565 (Fed. Cir. 1995).

often combined with enablement rejections, which scholars have attributed to inherent bias and more stringent examination against chemical-based inventions than predictable inventions.[127] Since the enablement and utility requirements are closely related, computational technological advancements require reassessing their interrelationships, which are described in more detail in Part IV.

IV. DOCTRINAL DISRUPTIONS BY COMPUTATIONAL EXPERIMENTATION

Computational technologies challenge how we think about enablement and utility patent law doctrines. Chemicals, compounds, and materials can be experimented upon *in silico*. The difference between traditional experimental results and hypothetical ones is increasingly difficult to distinguish technologically and in the patent examination process. As computational technologies continue to mature, patent law will need to respond to a research environment in which the worlds of laboratory and computational experimentation move closer together.

Some aspects of computational technologies fit comfortably within the patent law doctrine. For example, researchers are permitted to use tools for scientific research.[128] But patent law encounters difficulty with computational research tools[129] that create hypothetical structures, mask disclosure patentability requirements, or make it easier to file a patent application earlier than allowed within examination guidelines.

This Part highlights some doctrinal disruptions with computational technologies and US patent law. It creates a framework for analyzing doctrinal difficulties and introduces patent policy considerations that are addressed in Part V.

A. Should the Utility Requirement Be Strengthened?

A threshold doctrinal inquiry for computationally derived inventions is utility. The assessment of the scope of the utility doctrine in light of rapid development and adoption of computational research

127. *See* Seymore, *Making Patents Useful*, *supra* note 80, at 1048–49, 1068 (suggesting a bias against granting patents in the unpredictable arts).

128. *See* Ted Hagelin, *The Experimental Use Exemption to Patent Infringement*, 58 FLA. L. REV. 483, 510, 511 (2006).

129. *See* Lillian Ewing, In Re Fisher: *Denial of Patents for ESTs Signals Deeper Problems in the Utility Prong for Patentability*, 8 MINN. J.L. SCI. & TECH. 645, 663 (2007) (noting that since there is no bright line test to determine what constitutes a research tool and since the USPTO has not clearly defined what constitutes a research tool, then research tools can be a full range of tools that scientists use in the laboratory as suggested by a definition of the NIH).

capabilities is important for numerous reasons to inventors, the USPTO, and courts. One reason is that the definition of enablement is not met if utility is not met.[130] Therefore, understanding the scope of the utility requirement in the computational world lessens the need to assess another legal requirement and in doing so, lessens administrative and judicial resources. Another reason is that prior challenges at the USPTO and in courts suggest that utility will be heavily scrutinized in patent applications for nascent technologies and in unpredictable arts.[131] Yet another reason is to provide inventors greater clarity on the utility patentability requirement in order to incentivize them to seek patents rather than trade secret protection, which could lessen follow-on innovation.[132] These reasons motivate an understanding of the word, statute, and case law of utility and, in doing so, suggest how to assess utility for an example of an advanced computational technology.[133]

While section 101 of the Patent Act requires that patents only be issued to "useful" inventions,[134] it is less of an obstacle to the issuance of a patent in most fields compared to other patentability requirements.[135] However, utility can be a significant hurdle to patentability in the unpredictable arts[136] where chemicals and compounds are synthesized without precise application or knowledge of any particular working result.[137] Computational technologies, which enable *in silico* design[138] or parallel computational-synthetic development[139] of chemicals and compounds, could complicate determining utterly incredible inventions and those that should belong in the domain of meeting patentability. The utility requirement is

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130. *See Process Control Corp.*, 190 F.3d at 1358.

131. *See* Seymore, *Making Patents Useful*, *supra* note 80, at 1049.

132. *See* Simon & Sichelman, *supra* note 76, at 383, 417 (contending that data-generating technologies can produce trade secrets in distinct product markets and could extend deadweight losses to the same class of consumers).

133. *See infra* Section IV.A.2.

134. 35 U.S.C. § 101 (2018).

135. *See* Seymore, *Making Patents Useful*, *supra* note 80, at 1049–50.

136. *See id.*

137. *See id.* at 1053.

138. *See supra* note 6 and accompanying text.

139. *See* Sara Szymkuć et al., *Computer-Assisted Synthetic Planning: The End of the Beginning*, 55 ANGEWANDTE CHEMIE 5904, 5906 (2016) (noting that a combination of modern computational power and algorithms together with organic synthesis techniques optimizes pathways involving reactions); Derek Lowe, *The Algorithms Are Coming*, SCI. TRANSLATIONAL MED. (Apr. 12, 2016), https://blogs.sciencemag.org/pipeline/archives/2016/04/12/the-algorithms-are-coming [https://perma.cc/7XAA-FW3X] ("[M]odern computers can finally provide valuable help to practicing organic chemists. . . . [S]ynthesis-aiding programs . . . should be regarded precisely as 'chemical calculators,' accelerating and facilitating synthetic planning, rapidly offering multiple synthetic options which a human can then evaluate and perhaps improve in creative ways.").

meant to prevent mere ideas from being patented, but the advent of computational technologies makes it challenging to distinguish mere ideas from those possessing substantial and specific utility.

1. Utility in Early Patent Cases in the Unpredictable Arts

Early biotechnology and pharmaceutical chemistry patent cases[140] concerned the utility requirement for patentability. The context of these biochemical research cases involved research of chemical compounds without a particular purpose in mind.[141] The chemical researchers in these patent cases attempted to synthesize chemical compounds that they hoped would be useful for something, but did not know of a particular use at the time of synthesis.[142] Thus, the chemists were experimentalists, and they ran headlong into patent law's utility requirement as they filed patents claiming their synthesized chemical compounds. While they lacked the *in silico* design tools for early computationally derived development and analysis of their chemical compounds, these patent cases serve as predecessors to doctrinal assessment of current technological capabilities for predictive design of compounds with specified chemical properties.

In *Brenner*, the inventor, Manson, claimed a new process for making a known steroid. Manson asserted that his process had utility because the steroid that it produced was being screened for tumor-inhibiting effects in mice.[143] The issue involved whether utility is met for a chemical process that yields an already-known product whose utility has not been evidenced.[144] The Court held that utility was not satisfied because no specific benefit was shown since it was not demonstrated how the steroid served a practical function.[145] One underlying patent policy consideration by the *Brenner* Court is the

140. *See* Brenner v. Manson, 383 U.S. 519, 520 (1966); *In re* Fisher, 421 F.3d 1365, 1366–67 (Fed. Cir. 2005); *In re* Brana, 51 F.3d 1560, 1562 (Fed. Cir. 1995).

141. *See Brenner*, 383 U.S. at 520, 522–23; *Fisher*, 421 F.3d at 1367–68; In re *Brana*, 51 F.3d at 1562–63.

142. *See Brenner*, 383 U.S. at 522–23; *Fisher*, 421 F.3d at 1368; In re *Brana*, 51 F.3d at 1562–63.

143. *See Brenner*, 383 U.S. at 521–22 (noting that although the particular compound that the inventor Manson was concerned with was known in the art and of interest to the scientific community, chemists had yet to identify any setting in which it could be gainfully employed).

144. *See id.* at 532.

145. *See id.* ("[The patent applicant] did not disclose sufficient likelihood that the steroid yielded by his process would have similar tumor-inhibiting characteristics."); *id.* at 534–35 ("Until the process claim has been reduced to production of a product shown to be useful, the metes and bounds of that monopoly are not capable of precise delineation. . . . Unless and until a process is refined and developed to this point—where specific benefit exists in currently available form—there is insufficient justification for permitting an applicant to engross what may prove to be a broad field.").

possibility that having too stringent of a utility requirement would deter research by later inventors.[146]

The case *In re Brana* concerned chemical compounds that were useful as antitumor substances.[147] In that case, the USPTO Board of Patent Appeals and Interferences rejected the patent application for lack of utility due to tests being conducted upon lymphomas induced in laboratory animals rather than real diseases. The Federal Circuit reversed the rejection and held that an inventor does not need to wait until a disease appears in an animal or human before finding a cure to satisfy utility.[148] The Federal Circuit's view was that the evidence of utility did not require tests for full safety and effectiveness of the compounds.[149] Thus, one underlying patent policy consideration was the level of experimental evidence necessary to satisfy utility for patentability.[150]

The case *In re Fisher* involved expressed sequence tags and addressed whether utility was met where the patent specification did not disclose how to use the specific gene expression data.[151] The Federal Circuit held that utility was not met because the patent applicant simply provided a laundry list of research plans without any specific and substantial benefit.[152] The Federal Circuit pointed out that the claimed expressed sequence tags were no more than research intermediaries that were the objects of use-testing requiring further experimentation.[153] Therefore, one underlying patent policy consideration for evaluating utility was the extent to which experimental results are complete, rather than the intermediary step in research.[154]

The policy questions in the three aforementioned patent cases concerned the timing of patent grants, successful experimental

146. *See id.* at 533–34.

147. *In re* Brana, 51 F.3d 1560, 1562 (Fed. Cir. 1995).

148. *See id.* at 1563–64, 1565 (suggesting that one skilled in the art would be without basis to reasonably doubt the asserted utility on its face and that evidence of success in structurally similar compounds is relevant in determining whether one skilled in the art would believe an asserted utility).

149. *See id.* at 1567.

150. *See id.* at 1566–67.

151. *In re* Fisher, 421 F.3d 1365, 1367–69 (Fed. Cir. 2005) (nothing that the expressed sequence tags at issue encoded proteins and protein fragments in maize plants for a variety of uses, including controlling protein expression, monitoring gene expression, and serving as molecular markers).

152. *See id.* at 1373–74, 1376 (reasoning that until corresponding genes and proteins have a known function, then the claimed expressed sequence tags lack utility and that there were mere hypothetical possibilities since none of the expressed sequence tags were used in the real world).

153. *See id.* at 1373.

154. *See, e.g., id.*

evidentiary requirements, and level of intermediary-to-completion continuum in the nature of experiments. These patent cases suggest that progress in scientific research alone does not fulfill the utility requirement. The judicial resolution in these cases highlights that utility is not met when overly broad patent protection is sought beyond the scope of scientific achievement.

In response, large pharmaceutical companies have expressed concern that allowing patents on compounds and chemicals that are early in development and far from final marketable products would reduce industry growth.[155] The policy considerations in these early cases could be magnified even further with the advent and proliferation of computational experimentation. Pharmaceutical companies will be more motivated to tighten patentability requirements to make it more difficult to obtain early patent protection on computationally-derived inventions. The following application provides an example of policy impact, which could affect chemical research in materials science as well as in pharmaceuticals.

2. Application: Grand Canonical Monte Carlo Simulations of Metal Organic Frameworks

To illustrate the current utility framework being challenged by advancements in computational technology capabilities in the unpredictable arts, consider the following example. Suppose a researcher-inventor seeks to develop a chemical compound that would retard the ripening and ruining of fruit. The researcher-inventor knows that plant hormones released by a certain fruit will trigger ripening of that fruit and that a tailor-designed, absorbent nanocrystal would bind to enzymes in that fruit to block the effect of that hormone. The researcher-inventor could hire a patent attorney to conduct a prior art search[156] to identify desiccants[157] that were ineffective for that particular fruit or in blocking that hormone's effect in general. Although the researcher-inventor has not conducted any experiments on the proposed nanocrystal compound and does not possess access to

155. Brief of Genentech, Inc. as Amicus Curiae Supporting Affirmance and Supporting the United State Patent and Trademark Office (December 15, 2004); Brief for Amicus Curiae Affymetrix, Inc. In Support of Appellee (December 14, 2004); Brief for Amici Curiae by Eli Lilly and Company: In re Dane K. Fisher and Raghunath V. Lalgudi (December 14, 2004).

156. *See* Corinne Langinier & Phillipe Marcoul, *Search of Prior Art and Revelation of Information by Patent Applicants*, 49 REV. INDUST. ORG. 399, 401 (2016).

157. *More About Desiccants*, THOMAS PUB. COMPANY, https://www.thomasnet.com/about/desiccants-22064802.html [https://perma.cc/PVR6-TDR3] (defining desiccants as "drying agents that extract water from a wide range of materials") (last visited Jan. 16, 2019).

laboratory equipment for conducting such synthetic experiments, the researcher-inventor utilizes computational technology to predict properties of hypothetical nanocrystal compounds for retarding of fruit ripening. The researcher-inventor simulates millions of potential compounds within specified ranges of fruit ripening prevention characteristics that possess manufacturability characteristics, and selects underlying common chemical composition characteristics of the genus of compounds.[158] The researcher-inventor works alongside the patent attorney to file broad, prophetic examples[159] with composition of matter patent claims,[160] and prepares a specification based on the simulation results. Although the researcher-inventor has not conducted any synthetic experiments, the researcher-inventor is able to use computational technology to predict the nanocrystals' pore size, chemical composition, and absorption properties—each of which are written in the patent specification as if the researcher-inventor had conducted synthetic experiments. The patent attorney utilizes the researcher-inventor's tables and examples and files not only composition of matter patent claims,[161] but also method of manufacturing patent claims[162] and an apparatus patent claim[163] of a system comprising a storage container holding the nanocrystals.[164] The researcher-inventor may even commence some experiments if there are rejections in Office actions from the USPTO to quickly and effectively provide quick scientific input that may easily overcome the patent

158. *See* MPEP, *supra* note 13, § 2164.02.

159. *See id.*, § 2164.02; *see, e.g.*, Atlas Powder Co. v. E.I. du Pont de Nemours & Co. 750 F.2d 1569, 1577 (Fed. Cir. 1984); Freilich, *supra* note 24, at 53.

160. *See* Alan G. Towner, *Patenting Materials-Related Inventions*, 52 JOM 48, 48 (2000).

161. *See id.*

162. *See generally* ROBERT C. FABER, FABER ON MECHANICS OF PATENT CLAIM DRAFTING ch. 4 (7th ed. 2017).

163. *See id.* ch. 3.

164. There are strategic and business reasons why a patent attorney would file various types of independent patent claims with varying patent claim scope. For example, the issuance of such a system patent claim could prevent a distributor that is in the business of assembling chemical storage containers from entering a new business involving storage of such nanocrystals; in turn, the researcher-inventor, or the company to which the researcher-inventor's patents are assigned, could attain a lucrative licensing royalty stream form the storage container distributor. As an additional example, the issuance of a method of manufacturing patent claim could prevent a manufacturer that is in the business of processing chemicals from entering a new business involving manufacturing of such nanocrystals; in turn, the researcher-inventor, or the company to which the researcher-inventor's patents are assigned, could have leverage in the business relationship with such a manufacturing company. Thus, the researcher-inventor, or the research and development company to which the researcher-inventor's patents are assigned, could have added strategic business leverage with manufacturing companies and distribution companies by virtue of issuance of method of manufacturing patent claims and system patent claims.

examiner's arguments during the prosecution of the patent claims.[165] Thus, the computational technology is effective not only at the filing stage of the patent application, but also for responding to any utility (or enablement) rejections by the patent examiner during patent prosecution.

What type of computational technology provides such a result? And how can utility be viewed and potentially strengthened in light of such a computational capability? One such computational technology that could be utilized in the aforementioned illustrative example of computational experimentation involves Grand Canonical Monte Carlo (GCMC) simulations—a simulation type analogous to molecular dynamics simulations[166]—of metal organic frameworks (MOFs). Computational technologies assist in the design of MOFs, which are a "class of porous materials, made of metal clusters bound to organic molecules."[167] MOFs are crystalline materials characterized by an open framework, tunable pore size and functionality, and high surface area.[168] Since MOFs are akin to Lego-like building blocks, it is possible to create millions of MOF variations, each with particular characteristics and properties.[169] MOFs have existing commercial

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165. As an example, the patent application can reject be rejected for utility if the patent examiner considers that the prophetic examples of the hypothetical chemical structures for retarding fruit ripening does not meet the substantial and specific utility test. *See, e.g.*, Bos. Sci. Corp. v. Johnson & Johnson Inc., 679 F. Supp. 2d 539, 556–57 (D. Del. 2010). In an Office action response to the utility rejection, the patent attorney could utilize additional scientific, synthetic experimental chemistry understanding to overcome such a rejection. While no new matter can be introduced after the patent application is filed and while the patent attorney must utilize the content in the originally-filed patent application or make persuasive argument as to why the patent examiner is wrong, the patent attorney can gain an added understanding through synthesis experiments that could scientifically clarify the previously-filed invention that was computationally derived. *See supra* Section III.B. To be clearer, suppose that the computational technology helped to identify the correct combination of chemical components of the nanocrystal compound claimed in the originally-filed patent application, but that the resulting nanocrystal compound's properties were not know at the time of filing the patent application. The subsequent synthetic chemical experiments could provide clues about the physical properties of the nanocrystal compounds that the patent attorney could argue to overcome the patent examiner's view in the response to the Office action or could be better explained during an examiner interview.

166. *See* Allen, *supra* note 46, at 1 (noting the similarities in both molecular dynamics and monte carlo simulations while noting that molecular dynamics provide dynamical properties of the systems, such as transport coefficients, time-dependent responses to perturbations, and rheological properties).

167. *See* Hiroyasu Furukawa et al., *The Chemistry and Applications of Metal-Organic Frameworks*, 341 SCI. 974, 974 (2013); *Full of Hot Air and Proud of It: Improving Gas Storage with MOFs*, PHYS.ORG (Apr. 17, 2018), https://phys.org/news/2018-04-full-hot-air-proud-gas.html [https://perma.cc/5R7A-U8ZH].

168. *See* Chandan Dey et al., *Crystalline Metal-Organic Frameworks (MOFs): Synthesis, Structure, and Function*, 70 ACTA CRYSTALLOGRAPHICA 3, 3 (2014).

169. *See* Edwin Argueta et al., *Molecular Building Block-Based Electronic Charges for High-Throughput Screening of Metal-Organic Frameworks for Adsorption Applications*, 14 J. CHEMICAL THEORY & COMPUTATION 365, 365 (2018); Richard J. Gowers et al., *Automated Analysis*

use,[170] are sold by commercial distributors,[171] and have new applications in multi-billion dollar gas storage, gas separation, sensing, and catalysis applications and markets.[172] The modular nature of MOFs is particularly useful in GCMC simulations, since a researcher can "guess the structure of the not yet synthesized materials [by] using a systematic variation and assembly of the building blocks" in an iterative fashion.[173]

Such GCMC simulations can predict material characteristics, such as porosity and specific surface area,[174] and material properties, such as mechanical and thermal properties,[175] prior to any synthetic experiments.[176] Thus, materials science researchers can predict properties of potential functional materials before conducting any reduction to practice. A comprehensive library and database of nearly one million porous materials' crystal structures—many of them initially developed by computational research tools[177]—have been compiled in the Cambridge Structural Database.[178] GCMC simulations are creating more and more nanocrystal compounds for many types of applications,[179] such as the aforementioned retarding of fruit ripening illustration.

In light of the GCMC simulations, which are being utilized for many other use cases and commercial applications, should the utility

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and Benchmarking of GCMC Simulation Programs in Application to Gas Adsorption, 44 MOLECULAR SIMULATION 309, 309 (2017).

170. *See* Amarajothi Dhakshinamoorthy, Mercedes Alvaroa & Hermenegildo Garcia, *Commercial Metal-Organic Frameworks as Heterogeneous Catalysts*, 48 CHEMICAL COMM. 11275, 11277–78 (2012).

171. *See, e.g., Metal Organic Frameworks*, SIGMA-ALDRICH, https://www.sigmaaldrich.com/technical-documents/articles/materials-science/metal-organic-frameworks.html [https://perma.cc/GE4M-NHKB] (last visited Jan. 17, 2019).

172. *See* Bilge Yilmaz, Natalia Trukhan & Ulrich Müller, *Industrial Outlook on Zeolites and Metal Organic Frameworks*, 33 CHINESE J. CATALYSIS 3, 7 (2012).

173. *See* Gowers et al., *supra* note 169, at 309.

174. *See* Wen-Li Xie et al., *Grand Canonical Monte Carlo Simulation of Nitrogen Adsorption in a Silica Aerogel Model*, 4 COMPUTATION 18, 18 (2016).

175. *See* Francois-Xavier Coudert & Alain H. Fuchs, *Computational Characterization and Prediction of Metal-Organic Framework Properties*, 307 COORDINATION CHEMISTRY REV. 211, 219–22 (2015).

176. *See, e.g.*, Xie et al., *supra* note 174, at 2, 8 (stating that computational screening of materials can identify the best material for a particular application before the actual experimentation is committed through virtual screening strategies).

177. *See* Peyman Z. Moghadam et al., *Development of a Cambridge Structural Database Subset: A Collection of Metal-Organic Frameworks for Past, Present, and Future*, 29 CHEMISTRY MATERIALS 2618, 2618 (2017).

178. *The Cambridge Structural Database (CSD)*, CAMBRIDGE CRYSTALLOGRAPHIC DATA CTR., https://www.ccdc.cam.ac.uk/ [https://perma.cc/3SG8-BDKV] (last visited Jan. 17, 2019).

179. *See, e.g.*, Gowers et al., *supra* note 169; Attila Malasics, Dirk Gillespie & Dezső Boda, *Simulating Prescribed Particle Densities in the Grand Canonical Ensemble Using Iterative Algorithms*, 128 J. CHEMICAL PHYSICS 124102-1, at 1 (2008).

requirement in US patent law be strengthened? GCMC simulation capability provides an example of a capability that can predict material characteristics to meet the utility test, particularly the substantial and specific utility prong. In the aforementioned illustrative example, GCMC simulations can predict adsorption isotherms[180] with extremely high accuracy with experimental data[181]; therefore, GCMC simulations could satisfy the substantial and specific utility prongs by providing real world application and by demonstrating chemical and physical properties without synthetic experiments. In other words, since GCMC simulations can predictively discover nanocrystal structural, geometrical, physical, optical, and electronic properties through large-scale screening of hypothetical structures,[182] these unique properties applicable for large chemical groups could easily satisfy the utility requirement for patentability. GCMC simulations of MOF nanocrystals could also plausibly satisfy the elevated utility standard for research intermediaries[183] since the simulated MOFs are building blocks[184] and not intermediaries; moreover, such simulated MOFs would have uses specific to the claimed invention.

This example suggests that the current utility standard in US patent law has not kept pace with computational developments in the unpredictable arts.[185] In light of computational experimentation, the utility standard is vague[186] because it forces the patent applicant to prove specific uses, specific properties, and specific real world uses while still allowing for prophetic examples.[187] First, the current test for utility in US patent law fails because it is ill-suited for computational

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180. *See* Paul A. Webb, *Introduction to Chemical Adsorption Analytical Techniques and Their Application to Catalysis*, MIT TECHNICAL PUBLICATIONS 1, 1–2 (2003), http://www.micromeritics.com/Repository/Files/intro_to_chemical_adsorption.pdf [https://perma.cc/AR3N-4MXH] (defining a chemical adsorption isotherm as "the relationship between the quantity of molecules adsorbed and the pressure at constant temperature").

181. *See, e.g.*, Gowers et al., *supra* note 169, at 315.

182. *See* Coudert & Fuchs, *supra* note 175, at 212–22.

183. *See* Brenner v. Manson, 383 U.S. 519, 534–35 (1966) (articulating an elevated utility standard for research intermediaries and reasoning that an "object of use-testing" was insufficient to meet the utility requirement); *In re* Joly, 376 F.2d 906, 908 (C.C.P.A. 1967) (clarifying that simple use of an intermediate was not sufficient to show utility).

184. *See* Coudert & Fuchs, *supra* note 175, at 213–15 (noting that the Automated Assembly of Secondary Building Units method, or AASBU, produces auto-assembled three-dimensional frameworks).

185. *See* Ewing, *supra* note 129, at 664–65 (suggesting that the utility test stemming from *Brenner* and applied in *Fisher* is "unrealistic for research-relate inventions, which by their very nature encompass research into the unknown").

186. *See* Tashica T. Williams, In Re Fisher*: Raising the Utility Hurdle for Express Sequence Tags*, 21 BERKELEY TECH. L.J. 123, 124–25, 145 (2006) (noting that the *Fisher* case did not provide a precise standard for the minimum necessary utility by effectively conceptualizing a timeline tracking an invention's "ripeness").

187. *See* Freilich, *supra* note 24, at 1.

research tools. Second, the current test for utility fails to account for computational experimentation since such simulations can yield useful products and processes that independently satisfy utility, even if the output of computational simulations are hypothetical structures. This Article discusses each of these reasons in detail.[188]

B. Should the Enablement Requirement Be More Rigorous?

In the unpredictable arts, such as biotechnology, chemistry, and materials science, courts have generally been stricter in judging broadly defined patent claims.[189] Courts recognize that some degree of speculation is inherent in patent applications for the unpredictable arts.[190] Therefore, courts and the USPTO must assess patentability with a balance of a tolerable degree of speculation and of undue experimentation to practice the invention.

Computational capabilities magnify the challenge of assessing whether a given specification requires undue experimentation to produce the embodiments. The *Wands* factors,[191] which continue to be utilized in assessing whether enablement is met, are misplaced and inapplicable in modern research where computational capabilities are pervasive. The *Wands* factors assessment was formulated at a time of only synthetic research capabilities and does not consider the presence of computational capabilities in determining whether a disclosure would require undue experimentation. While there is latitude in some of the *Wands* factors, such as the quantity of experimentation necessary,[192] the *Wands* factors are based on assessment from a synthetic experimentation without consideration of computational capabilities.

Thus, a reevaluation of the speculation-experimentation balance of the enablement doctrine requires consideration of computational capabilities. An assessment of whether and how computational capabilities complicate enablement and undue experimentation starts with review of early patent cases concerning speculation and prophesy. The patent policy dilemmas concerning enablement from the early

188. *See supra* Sections IV.A.1.

189. *See* Res., Inc. v. Roxane Labs., Inc., 253 F. App'x 26, 30 (Fed. Cir. 2007); Seymore, *Enablement Pendulum*, *supra* note 72, at 282, 292 (pointing out that an inventor need not disclose every embodiment at the time of filing and that some of the disclosure standard is based on speculation in the unpredictable arts). *But see* Ouellette, *supra* note 22, at 1832 (noting the presence of "speculative disclosures" in unpredictable technologies).

190. *See* Seymore, *Heightened Enablement*, *supra* note 1, at 144.

191. *See In re Wands*, 858 F.2d 731, 737 (Fed. Cir. 1988).

192. *See* Amgen, Inc. v. Chugai Pharm. Co., 927 F.2d 1200, 1213 (Fed. Cir. 1991); *In re Wands*, 858 F.2d at 737 (factor 1).

patent cases discuss issues from a synthetic experimentation lens that should expand to involve assessment from a computational lens.

1. Enablement in Early Patent Cases in the Unpredictable Arts

In addition to the early patent cases in the unpredictable arts concerning the utility requirement,[193] there exist similar cases related to the enablement requirement. *Janssen Pharmaceutica N.V. v. Teva Pharmaceuticals USA* involved issues related to enablement and utility in relation to a patent with a claim directed to a method for treating Alzheimer's disease with a pharmaceutical compound.[194] The patent assignee, Janssen Pharmaceutica, sued manufacturers for infringement of its patent. The district court concluded that the patent at issue was invalid for lack of enablement.[195] On appeal, the Federal Circuit concluded that the specification simply stated a hypothesis and proposed testing to determine its accuracy, which was insufficient to meet enablement.[196] The appellate court concluded that since utility of galantamine as a treatment for Alzheimer's could not be established by a PHOSITA, enablement could not be met.[197] The court came to this determination by connecting enablement and utility doctrines through citing another case, which stated that "[i]f a patent claim fails to meet the utility requirement because it not useful or operative, then it also fails to meet the how-to-use aspect of the enablement requirement."[198]

Ariad Pharmaceuticals, Inc. v. Eli Lilly & Co. also involved a chemical case concerning molecules capable of particular chemical

193. *See* Brenner v. Manson, 383 U.S. 519, 528–29 (1966); *In re* Fisher, 421 F.3d 1365, 1370, 1373 (Fed. Cir. 2005); *In re* Brana, 51 F.3d 1560, 1564 (Fed. Cir. 1995).

194. Janssen Pharmaceutica N.V. v. Teva Pharms. USA, Inc., 583 F.3d 1317, 1320–23 (Fed. Cir. 2009).

195. *Id.* at 1323 (justifying enablement not being met on two grounds: first, the district court determined that the specification did not meet utility because relevant animal testing experiments were not completed by the time that the patent was issued and the specification contained minimal utility; second, the district court concluded that the specification did not "'teach one of skill in the art how to use the claimed method' because the application 'only surmise[d] how the claimed method could be used' without providing sufficient galantamine dosage information . . . .").

196. *Id.* at 1321–22, 1327 (pointing out that the patent specification was only about one page in length and did not refer to any test results involving the administration of galantamine in connection with Alzheimer's disease and that statements by the patent applicant, indicating that "experiments [are] underway" and that it was "expected that data from this experimental work will be available," suggested a mere idea (internal quotation marks omitted) (alteration in original)).

197. *Id.* at 1327.

198. *Id.* at 1323–24 (citing Process Control Corp. v. HydReclaim Corp., 190 F.3d 1350, 1358 (Fed. Cir. 1999)).

activities.[199] The asserted patent claims were genus claims, and the patent specification hypothesized molecules for reducing particular chemical activities in cells.[200] The Federal Circuit reaffirmed the written description requirement and further noted that there must be possession of the claimed methods to satisfy the written description requirement by sufficiently disclosing the molecules' activity.[201] One reading of the court's reasoning is that there is a notable difference between describing an invention and teaching about it and that a generic claim may only define a vast genus of chemical compounds when the applicant demonstrates possession of the claimed invention. The USPTO issued patent examination guidance concerning the "possession test" and required "sufficient evidence of possession [such as] the level of skill and knowledge in the art, partial structure, physical and/or chemical properties, functional characteristics alone or coupled with a known or disclosed correlation between structure and function, and the method of making the claimed invention."[202] Legal scholars also proposed ways to demonstrate "possession"[203] and elaborated on what "possession" of an invention meant for disclosure.[204] Therefore, one underlying patent policy consideration was how broadly an inventor could attempt to capture claims in the patent, as compared to the amount of teaching shown or possession demonstrated in the patent specification.

The policy questions in the two aforementioned patent cases concerned whether there was early disclosure at the time of filing the patent application, whether the inventor invented the species to support a claim to the genus, and whether the patent satisfied the written description requirement even if enablement was met. These

199. Ariad Pharms., Inc. v. Eli Lilly & Co., 598 F.3d 1336, 1340, 1354 (Fed. Cir. 2010) (en banc) (concerning regulation of mechanisms by which NF-kB "activates gene expression underlying the body's immune response to infection").

200. *Id.* at 1341, 1354 (explaining how the genus patent claims corresponded to the use of all substances that achieved the binding of NF-kB to NF-kB recognition sites, and the patent specification hypothesized NF-kB reduction activity in cells with three types of molecules).

201. *Id.* at 1355 (noting that the mere use of the three classes of molecules to achieve NF-kB reduction was insufficient disclosure, and instead, the applicant must "satisfy the inventor's obligation to disclose the technologic knowledge upon which the patent is based, and to demonstrate that the patentee was in possession of the invention that it claimed").

202. MPEP, *supra* note 13, § 2163 ("Disclosure of any combination of such identifying characteristics that distinguish the claimed invention from other materials and would lead one of skill in the art to the conclusion that the applicant was in possession of the claimed species is sufficient.").

203. *See* Holbrook, *supra* note 22, at 147 (proposing enablement as the best mechanism to demonstrate possession).

204. Christopher A. Cotropia, *Claim Interpretation and Information Costs*, 9 LEWIS & CLARK L. REV. 57, 68–69 (2005) (concluding that written description requires inventor to disclose the universe of potential embodiments he or she may ultimately claim).

patent cases suggest that the patent specification must demonstrate "possession," which is intangible but will be satisfied when enablement is met.[205] The judicial resolution in these cases highlights that enablement is not met when overly broad patent protection is sought because the specification does not demonstrate inventor's possession or another could not make the invention without undue experimentation.

2. Application: Computationally Created Chemical Intermediaries

Unlike MOFs, which are akin to assembled Lego-like building blocks that can connect into larger chemical frameworks later,[206] chemical intermediaries react further to create products as a result of a chemical reaction. To illustrate the challenges the current enablement framework faces from advancements in computational technology capabilities, consider the following example. Suppose a researcher-inventor seeks to develop a new protein supplement bar for canines.[207] The researcher-inventor is skilled in the art of developing protein bars for humans and is employed by a sports nutrition company that has knowledge of recent research on nutrition for canine athletes. The researcher-inventor's employer has determined there are only a few existing canine protein bars on the market[208] and that the company can develop better and more effective canine protein bars. The researcher-inventor has conducted numerous synthetic chemistry experiments to identify the correct formulations for prior product launches of protein bars for humans. Additionally, the researcher-inventor seeks a faster research and development method for identifying the optimal formulation for protein bars for canines to gain a competitive advantage in the new canine nutrition marketplace. The researcher-inventor's employer recognizes that computational protein design can predict the

205. *See* Holbrook, *supra* note 22, at 146–47 (stating that the "thing" possessed, however, is intangible and that possession must be demonstrated to communicate to the world what the inventor created; suggesting that the key aspect of possession is determining whether or not one can make a functional device; and concluding that the best evidence of possession is either the inventor demonstrating that he/she has physically created the invention or has provided a description that would allow someone else in the art to physically create the invention).

206. *See* Argueta et al., *supra* note 169, at 366.

207. *See* Gretchen Reynolds, *Feeding Your Canine Athlete*, N.Y. TIMES (Aug. 20, 2014, 12:01 AM), https://well.blogs.nytimes.com/2014/08/20/the-science-behind-your-dogs-special-exercise-needs/ [http://perma.cc/GP6Z-BUFT] (showing that, while there are numerous protein bars for humans, there is a new and growing market of protein supplements for canine athletes, which have different biological and nutritional needs than human athletes).

208. *See, e.g.*, HULKBAR, https://bullymax.com/hulkbars [https://perma.cc/C8W3-ZVHU] (last visited Jan. 28, 2019); MUSCLE BULLY PROTEIN, https://www.musclebully.com/products/dogprotein?variant=27792849670 [https://perma.cc/AJ6Q-AEBM] (last visited Jan. 28, 2019).

probability of structural properties in protein bars,[209] and accordingly hires a computational scientist to work alongside the researcher-inventor for a canine protein bar research and development project. Together, the research-inventor and the computational scientist utilize machine learning techniques[210] for predicting the probability of natural amino acids on each residue in a protein.[211] In order to predict the results of new reactions of the specialized chemicals necessary for effective digestion and absorption in canines following exercise, the machine learning algorithm utilizes information from human-relevant chemistry reactions that have been trained upon for canine-relevant chemistry reactions that it has yet to encounter.[212]

Similar to the use of machine learning in other organic chemistry reactions,[213] the research-inventor and computational scientist work together to predict properties of organic molecules based on the presence of functional key groups in the chemistry of protein bars. While the researcher-inventor and computational scientist develop their machine learning model, they generate a library of chemicals and reactions utilized in other protein bar chemistry applications for humans and carry out a few simple synthetic experiments of protein bar chemistry for canines. These efforts yield chemical intermediaries necessary in canine protein bars. The researcher-inventor and computational scientist work alongside a patent attorney to file broad genus patent claims covering a class of proteins for use in canine protein bars that will be formed from these chemical intermediaries and are specific to canine digestion and absorption.

The researcher-inventor, however, has yet to carry out any experiments of specific species of such proteins for use in canine protein bars. It is debatable how to demonstrate to a PHOSITA to make the protein for use in canine protein bars, as well as whether the patent specification provides partial structure, physical or chemical properties, and functional characteristics alone or coupled with a known or disclosed correlation between structure and function. Machine learning computational technology is effective for demonstrating enablement for

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209. Jingxue Wang et al., *Computational Protein Design with Deep Learning Neural Networks*, 8 SCI. REP. 6349, at 1 (2018), https://www.ncbi.nlm.nih.gov/pmc/articles/PMC5910428/pdf/41598_2018_Article_24760.pdf [https://perma.cc/4PU8-8D5X].

210. *See supra* Section II.B.

211. *See* Wang et al., *supra* note 209, at 1.

212. *See supra* Section II.B.

213. Jennifer N. Wei, David Duvenaud & Alán Aspuru-Guzik, *Neural Networks for the Prediction of Organic Chemistry Reactions*, 2 ACS CENT. SCI. 725, 726 (2016) (describing the use of neural networks for predicting reaction types, which, using a set of reagents and reactants, predicts the likely products).

a broad genus of chemical intermediaries of proteins for use in canine protein bars. How can machine learning technology provide such a result? And how should enablement be viewed and potentially be made more rigorous in light of such a computational capability?

Machine learning could be utilized in the aforementioned illustrative example of computational experimentation of chemical intermediaries for development of canine protein bars. Machine learning can sample and optimize millions of sequences that are likely to fold into desired protein structures given the protein backbone structure.[214] Thus, chemical researchers can predict the results of reactions of chemical intermediaries to guess the outcome of the reaction[215] and, in doing so, can enable researchers to pursue broad genus patent claims capturing the results of such reactions without actually conducting reactions. In other words, since machine learning can predictively discover reaction products, then broad genus patent claims could satisfy the enablement requirement for patentability by providing representative species in the embodiment without conducting experiments.

This example suggests that the current enablement standard in US patent law is ill-suited for the unpredictable arts in a world of computational experimentation.[216] Even though the mere existence of undue experimentation allows for some experimentation,[217] the criteria is immeasurable and computational capabilities make it even more difficult to determine whether a skilled artisan's hypothesized effort to make what is in the disclosure is too much. Thus, computational capabilities complicate the subjective predictability factor of the *Wands* factors.[218]

C. Is the Enablement Requirement Subsumed into the Utility Requirement?

In US patent law, if utility is not met, then enablement cannot be met either.[219] However, if a patent applicant has disclosed a substantial and specific utility, that fact alone does not provide a basis for concluding that the patent claims comply with the enablement

214. *See* Wang et al., *supra* note 209, at 2, 8–9.

215. *See* Wei, Duvenaud & Aspuru-Guzik, *supra* note 213, at 726.

216. Ewing, *supra* note 129, at 664–65 (suggesting that the utility test stemming from *Brenner* and applied in *Fisher* is "unrealistic for research-related inventions, which by their very nature encompass research into the unknown").

217. *See* Vetter, *supra* note 23, at 778.

218. *See In re Wands*, 858 F.2d 731, 737 (Fed. Cir. 1988).

219. *See* Process Control Corp. v. HydReclaim Corp., 190 F.3d 1350, 1358 (Fed. Cir. 1999).

requirement.[220] Utility and enablement are two separate patentability requirements,[221] and the Manual of Patent Examining Procedure also specifies that rejections for utility and enablement should be imposed separately.[222]

This Article asserts that the enablement requirement gets subsumed into the utility requirement for computationally derived inventions. Scholars have supported this Article's claim that the utility and enablement requirements are merging, and have pointed out that these doctrines are often confused yet critically important for the unpredictable arts.[223] Moreover, the Federal Circuit has validated this Article's concerns by stating that the "[l]ack of enablement and utility are closely related grounds."[224] In fact, these patentability requirements are not only closely related; particularly, the requirements are conceptually overlapping and act as a single requirement for computationally derived inventions. In practice, the current technology-neutral, unified patent system[225] divides into separate standards for computationally derived inventions and noncomputationally derived inventions. The differential application of patent standards to the computational world of invention promotes the need for new, technologically-specific patent legislation.[226] A number of factors caution against technology-specific tailoring of the patent system, including legal, economic, administrative cost, and narrow-mindedness.[227] A patent system where there is not clear demarcation of utility and enablement as patentability requirements would be detrimental to society.

220. MPEP, *supra* note 13, § 2164.07.

221. 35 U.S.C. §§ 101, 112.

222. MPEP, *supra* note 13, § 2164.07.

223. Jacob S. Sherkow, *Patent Law's Reproducibility Paradox*, 66 DUKE L. J. 845, 878, 882 (2017) (describing that utility inquires whether an invention is theoretically possible and not whether it is consistently possible and that some courts have merged the two doctrines to claim that some inventions are largely irreproducible but possible).

224. *See Process Control Corp.*, 190 F.3d at 1358.

225. Dan L. Burk & Mark A. Lemley, *Is Patent Law Technology-Specific?*, 17 BERKELEY TECH. L.J. 1155, 1156 (2002) (stating that, while patent law standards are designed to be flexibly adapted and be unified across technologies, recent jurisprudence suggests increasing divergence between the rules and the application of the rules to different technology industries).

226. *But see* Dan L. Burk & Mark A. Lemley, *Policy Levers in Patent Law*, 89 VA. L. REV. 1575, 1578–79, 1630 (2003) (suggesting that patent law should not jettison its uniform patent system to protect specific technologies and industries, which would lead to a need to develop different patent statutes and rights for each technology industry).

227. *Id.* at 1634–36 (reasoning against technology-specific and industry-specific tailoring of the patent laws on the basis of international legal barriers, economic theory, substantial administrative costs and uncertainty for Congress and district court judges, and narrow-minded thinking in not anticipating and not accommodating eventual changes in technology).

Computational technologies raise issues that suggest the utility standard is too weak and should be strengthened[228] and that the enablement standard is unclear and should be strengthened.[229] For example, the discussion of GCMC simulations of MOFs shows that the substantial and specific utility prongs can be satisfied by demonstrating chemical and physical properties without synthetic experiments.[230] As another example, the computationally created chemical intermediaries in the research and development of hypothetical canine protein bars demonstrates the enablement of broad genus patent claims without synthetic experiments.[231]

The current weak utility requirement and unclear enablement requirement for computationally derived inventions suggests that enablement is subsumed into utility. As proof, patent law requires that a lack of utility means enablement is not met.[232] In other words, if an invention is not considered "useful," then there is no need to explain how to make or use the invention. Moreover, if a PHOSITA in unable to make a chemical compound, then it is more likely than not that invention will not meet utility. For example, computationally created, hypothetical chemical structures unreproducible by a synthetic chemist are more likely than not to fail to meet utility. This can be illustrated through application in the earlier example, for which claims of machine learning created chemical intermediaries for canine protein bars (based on data sets of human protein bar properties)[233] may not meet the enablement requirement due to not meeting utility when a synthetic chemist produces final chemical products with effective digestive and adsorptive properties. In turn, substantial and specific utility may not be met due to a lack of real-world application when not applicable to either human or canine protein bars. In sum, for computationally created inventions of the unpredictable arts, the enablement requirement becomes subsumed into the utility requirement.

D. Rethinking Utility in a Computational World

The advent, rapid rise, and growing use of computational research tools in the unpredictable arts has caused doctrinal patent law disruptions to the utility and enablement doctrines.[234] This Article's

228. *See supra* Section IV.A.
229. *See supra* Section IV.B.
230. *See supra* Section IV.A.2.
231. *See supra* Section IV.B.2.
232. *See* Process Control Corp. v. HydReclaim Corp., 190 F.3d 1350, 1358 (Fed. Cir. 1999).
233. *See supra* Section IV.B.2.
234. *See supra* Section IV.A, IV.B.

claim that the enablement requirement is subsumed into the utility requirement for computationally derived inventions[235] requires a re-evaluation of the utility doctrine as computational research proliferates. There have been three major prior proposals concerning the utility doctrine: (1) eliminating utility as a patentability requirement, (2) changing the burden to require the patent applicant to prove utility, and (3) requiring commercial utility.

First, one proposal suggests that the utility requirement for patentability be eliminated, since it comes at a cost by being subjective, superfluous, and indifferent to the technical substance of the disclosure.[236] There exists an inherent bias and subjective assessment with the utility standard as some inventions meet utility with minimum explanation and others require more stringent explanation. This proposal suggests that the utility requirement is not necessary since the other patentability requirements effectively ensure that a patent provides the public with useful disclosure.[237] However, the elimination of the utility requirement would modulate the gatekeeping function of patentability to be acquiescent and allow for purely hypothetical[238] and incredible inventions[239] in the patent system. The elimination of the utility requirement and the resulting less strict patentability requirements[240] could increase patenting of computationally derived inventions of hypothetical chemical compounds and, in doing so, block chemical innovation by laboratory and synthetic chemistry companies.

Second, another proposal suggests reallocating the burden of persuasion of utility to the patent applicant, rather than the patent

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235. *See supra* Section IV.C.

236. *See* Seymore, *Foresight Bias*, *supra* note 73, at 1113 (proposing that removing utility from patentability would eliminate foresight bias in the unpredictable arts, and result in a win-win for the patent applicant, society, and the US patent system); Seymore, *Making Patents Useful*, *supra* note 80, at 1076–80 (suggesting that the current utility requirement is substantively bankrupt, since it remains as a matter of judicial interpretation, fosters secrecy, and promotes inventors to develop simple uses, and therefore, for these reasons, should have no place in the US patent system; further arguing that concealment and delayed disclosure hinders innovation).

237. Seymore, *Foresight Bias*, *supra* note 73, at 1113.

238. Guillaume Maurin, *Role of Molecular Simulations in the Structure Exploration of Metal-Organic Frameworks: Illustrations Through Recent Advances in the Field*, 19 COMPTES RENDUS CHIMIE 207, 208, 210 (2016) (noting that a huge collection of hypothetical MOFs have been predicted but only rarely synthesized so far; pointing out that a research group has generated more than 130,000 hypothetical MOFs); Seymore, *Foreseight Bias*, *supra* note 73, at 1111; *see also* *Hypothetical Metal-Organic Frameworks Database*, NW. UNIV. (2011), http://hmofs.northwestern.edu/hc/crystals.php [https://perma.cc/2SEL-FT5S] (providing a database of hypothetical chemical structures, which may or may not able to synthesized and which may or may not have been compared between to see if computational and synthesis align).

239. *See In re* Citron, 325 F.2d 248, 252–53 (C.C.P.A. 1963); MPEP, *supra* note 13, § 2107.01.

240. *See* Brenner v. Manson, 383 U.S. 519, 534 (1966); Seymore, *Foresight Bias*, *supra* note 73, at 1112.

examiner, since the inventor theoretically has superior information about the invention.[241] This proposal justifies reallocation of the current patentability presumption, where the patent applicant is rebuttably presumed to comply with utility at the time of filing of the patent application,[242] based on normative justifications.[243] In US patent law, a lack-of-utility rejection triggers an evidentiary burden-shifting process, in which the burden shifts to the applicant once the examiner has established a prima facie case of unpatentability.[244] The proposal to shift the utility burden to the patent applicant would place a tremendous burden on inventors in the unpredictable arts, who would instead seek trade secret protection,[245] which has been a sought-out protection in such scenarios.[246] Inventors in the unpredictable arts who seek patents for inventions of early-stage research would face long patent prosecution timelines and higher patent preparation legal bills to persuade the USPTO that utility is met during Office action responses. Moreover, the fundamental assumption that the burden of persuasion should reside with the party possessing superior information[247] over calculates the degree of superiority of such information. Inventors in the unpredictable arts may have only slightly superior information, since their inventions are in the early stages of research and development, and they may still be attempting to garner information on their discoveries.[248]

Third, a different proposal suggests that the utility requirement be modified to a direct commercial utility standard with two prongs, which would require sufficient evidence to convince a PHOSITA that: "a) there is a market for the invention, and that b) the invention can be manufactured at a cost sufficient to fulfill market demand."[249] While

241. *See* Seymore, *The Presumption of Patentability*, *supra* note 83, at 1033–36 (suggesting that the burden of persuasion should be assigned to a party if it has superior information needed to prove an issue, even if that party does not bear the initial burden of producing evidence).

242. *Id.* at 995, 997 (noting that a basic tenant of patent examination is that an applicant is entitled to a patent unless the USPTO can prove otherwise, meaning that the burden of proving patentability rests with the USPTO).

243. *Id.* at 1035–36 (suggesting for reallocation justifications that the applicant has superior information, that the USPTO has limited resources, and that federal courts have the power to do so based on good policy due to the absence of direction from Congress).

244. *See* Seymore, *Foresight Bias*, *supra* note 73, at 1125.

245. *See* Kewanee Oil Co. v. Bicron Corp., 416 U.S. 470, 482, 485, 487, 489 (1974); Michael Risch, *Why Do We Have Trade Secrets?*, 11 MARQ. INTELL. PROP. L. REV. 1, 11, 42, 62 (2007).

246. *See* Simon & Sichelman, *supra* note 76, at 387–90.

247. *See* Seymore, *The Presumption of Patentability*, *supra* note 83, at 1034–35.

248. *See* Simon & Sichelman, *supra* note 76, at 389–90; Seymore, *Heightened Enablement*, *supra* note 1, at 137.

249. Risch, *supra* note 79, at 1240–42 (further describing the two-pronged standard as: first, requiring that some group of people would want to purchase the invention; second, requiring

this commercial utility proposal comes closest to the economic definition of utility,[250] it also raises doctrinal and practical concerns. One problem with the commercial utility test is that it would create some overlap between market demand and practical utility,[251] such that it would be difficult to assess satisfaction of these requirements by inventors, the patent attorneys who represent them, and the USPTO during patent examination. The potential overlap between practical utility and commercial utility suggests that much of this new test could be captured by the current utility patentability requirement. Another problem with consumer utility is determining consumers' willingness to pay for a product,[252] as it would be a challenge to ascertain the market demand in the first prong of this proposed test. A major problem with the proposed consumer utility is that it is biased against inventions of the unpredictable arts, and even more biased against computationally derived inventions in the unpredictable arts. Since inventions in the unpredictable arts are earlier in their market development than other fields, they are far away from commercial application and disconnected from market demand. Thus, such a commercial utility standard would be a stringent requirement against inventions in the unpredictable arts[253] and would decrease incentives for inventors to computationally design chemical compounds.

Each of the prior proposals for the utility requirement modulate patentability and have shortcomings. The proposals vary on the tradeoff: Some proposals incentivize more pre-filing work for a more robust disclosure, but do so at the expense of earlier disclosure. Conversely, other proposals sacrifice the quality of disclosure.[254] The policy tradeoff is early disclosure versus stimulating innovation.[255]

V. REFORM PROPOSALS AND INNOVATION POLICY CONSIDERATIONS

An assessment of whether the utility requirement should be strengthened in response to computational capabilities[256] is a patent

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evidence that the cost of producing the invention would not prevent near-term market demand from being satisfied).

250. *Id.* at 1199, 1242 (defining consumer surplus as the difference between the amount consumers are willing to pay for a good and the price they actually pay; specifying that the first prong of the test represents the amount consumers are willing to pay, and the second prong of the test represents the price that suppliers are willing to accept).

251. *Id.* at 1246.

252. *See id.*

253. *See* Timothy R. Holbrook, *Patent Disclosures and Time*, 69 VAND. L. REV. 1459, 1486–87 (2016); Seymore, *Heightened Enablement*, *supra* note 1, at 137.

254. *See* Seymore, *Uninformative Patents*, *supra* note 96, at 393–95, 398–99.

255. *See supra* Section IV.C.

256. *See supra* Section IV.D.

policy question. The utility requirement for patentability should be assessed in light of the following related issues: (1) disclosure by the patent applicant and (2) verification by the USPTO of the sufficiency of the disclosure. Each of these facets concerning disclosure influences industries involving advanced materials, biotechnology compounds, and pharmaceuticals, where researchers must expend considerable efforts in synthesis[257] and analytical chemistry[258] before a viable material or compound can be marketed.

First, disclosure is the quid pro quo of US patent law and involves issues of timing and sufficiency.[259] The disclosure requirement affects the incentives[260] for chemical researchers—both synthetic and computational—to obtain patent protection on chemical-related products and processes. A strong disclosure requirement will prohibit chemical and computational researchers—and the organizations that employ them—from filing patent applications too early to avoid obstacles with the utility requirement[261] and the enablement requirement.[262] A weak disclosure requirement will incentivize chemical and computational researchers—as well as the organizations that employ them—to seek early granting of patents in order to obtain competitive advantage in the marketplace.[263]

Patent policy concerns should determine the depth, strength or weakness, and specificity of the utility requirement for computationally derived inventions. As a result, patent policy drives inventors' research and development efforts toward fulfilling the utility standard, as well as consideration of alternatives to patent protection. One way to address the phenomena of computationally derived inventions in the unpredictable arts is to strengthen the utility requirement in order to avoid enablement being subsumed into utility.[264] This will retain

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257. *See* Vu, Quyen & Huong, *supra* note 6, at 60–61.

258. *Analytical Chemistry*, AM. CHEMICAL SOC'Y (ACS), https://www.acs.org/content/acs/en/careers/college-to-career/areas-of-chemistry/analytical-chemistry.html [https://perma.cc/2U8U-ZCHE] (last visited Jan. 28, 2019) (defining analytical chemistry as "the science of obtaining, processing, and communicating information about the composition and structure of matter," involving the knowledge of measurement and instrumentation, separation based on different chemical properties, and interpreting and communicating data).

259. *See* J.E.M. Ag Supply, Inc. v. Pioneer Hi-Bred Int'l, Inc., 534 U.S. 124, 142 (2001).

260. Suzanne Scotchmer & Jerry Green, *Novelty and Disclosure in Patent Law*, 21 RAND J. ECON. 131, 132 (1990) (pointing out that the reason to grant patent protection is that it creates incentives to do research).

261. *See supra* Section IV.D.

262. *See supra* Section IV.B.2.

263. Stuart J.H. Graham et al., *High Technology Entrepreneurs and the Patent System: Results of the 2008 Berkeley Patent Survey*, 24 BERKELEY TECH. L.J. 1255, 1288 (2009) (summarizing survey results that demonstrate patents serve to promote startups' and large companies' competitive advantage).

264. *See supra* Section IV.C.

separate and distinct enablement and utility doctrines as is present with other technology applications. This Article makes the normative claim that applications for computationally derived inventions should be required to provide a laboratory-based working example to demonstrate utility.[265] While some critics may argue that such a heightened standard diverges from technology neutrality espoused by US patent law, scholars have commented that technology neutrality in US patent law is an outdated theoretical notion, and there is increasing divergence between rules and the application of rules to different technological industries.[266]

Second, patent examination includes checking the sufficiency of disclosure and of the procedural requirements towards patentability during a negotiation process between a patent examiner and a patent applicant.[267] The US patent examination process is a function of rules and standards promulgated by the US Supreme Court, the US Court of Appeals for the Federal Circuit, and the US Congress.[268] The Commissioner of Patents' Guidance informs patent examiners on interpretations of the rules and standards for patent examination.[269] The USPTO internal metrics also influence the patent examination process, particularly patent examiners' performance and ability to issue patents.[270] Moreover, patent examiner hiring norms and training affect the skill and attention paid to patent applications during the patent examination process.[271] Patent policy concerning disclosure is

265. *See infra* Section V.A.

266. Burk & Lemley, *supra* note 225, at 1156, 1183–85 (stating while the patent statute does not distinguish between different technological settings for applying legal standards, in practice there is technological-specificity in rule application and divergent standards; providing as evidence the dramatic differences in applying the same legal rules depending on the technology at issue and concluding the presence of industry-specific precedent from case to case).

267. Mark A. Lemley & Bhaven Sampat, *Examining Patent Examination*, 2010 STAN. TECH. L. REV. 2, 6 (2010); *see also* BRENT. A. OLSON, MINNESOTA PRACTICE SERIES: ADVANCED TOPICS IN BUSINESS LAW § 17.9 (2018).

268. John M. Golden, *The USPTO's Soft Power: Who Needs Chevron Deference?*, 66 SMU L. REV. 541, 544–45 (2013) (stating that the USPTO engages in some sort of interpretation of statutory language or judicial precedents, but that the USPTO lacks the capacity to issue binding substantive rules).

269. U.S. PATENT & TRADEMARK OFFICE, EXAMINATION GUIDANCE AND TRAINING MATERIALS, https://www.uspto.gov/patent/laws-and-regulations/examination-policy/examination-guidance-and-training-materials [https://perma.cc/G2XZ-2EQZ] (last visited Jan. 28, 2019).

270. Mark A. Lemley & Bhaven Sampat, *Examiner Characteristics and Patent Office Outcomes*, 94 REV. ECON. & STAT. 817, 818 (2012) (stating that patent examiners' incentives, such as their promotion and bonus decisions, are connected to "counts," which can occur based on a grant or disposal of a patent application and not by other patent examiner activities, which can include prior art searching and issuance of final rejections).

271. Iain M. Cockburn et al., *Are All Patent Examiners Equal?: The Impact of Characteristics on Patent Statistics and Litigation Outcomes* 8 (Nat'l Bureau of Econ. Research, Working Paper No. 8980, 2002).

intertwined with patent examination, which is an evaluation of the disclosure. Another way to address the phenomena of computationally derived inventions in the unpredictable arts is to improve patent examination of detection and assessment. This Article makes the normative claim that the USPTO should change patent examiner hiring norms and training for examination of computationally derived inventions.[272]

A. Requiring a Laboratory-Based Working Example in the Unpredictable Arts

The utility requirement for patentability requires both substantial and specific utility.[273] It also requires that inventions not be incredible.[274] However, experiments in patent applications may be fictional, and inventors are allowed to speculate with fictional data when filing a US patent application.[275] Inventors in the unpredictable arts, such as chemicals and pharmaceuticals, often do not reveal how or why their complex invention works since such information is neither discernable by inspection nor by reverse engineering.[276] In effect, US patent law equates such fictional data to factual data.[277] Inventors can meet patentability by claiming large chemical groups with utility that corresponds to specific biological, physical, or chemical properties,[278] even without conducting any synthetic chemistry experiments. Computational research capabilities, such as GCMC simulations, enable researchers to predict and potentially claim properties of chemical compounds, such as MOFs,[279] and such capabilities have been explained in computational research studies, as shown:

> We demonstrate a computational approach to generate all conceivable MOFs from a given library of building blocks (based on the structures of known MOFs) and rapidly screen them to find the best candidates for a specific application. From a library of 102 building blocks we generated 137,953 *hypothetical* MOFs and for each one calculated the pore-size distribution, surface area and methane-storage capacity. We

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272. *See infra* Section V.B.

273. *See* Seymore, *Making Patents Useful*, *supra* note 80, at 1066–67.

274. *See In re* Citron, 325 F.2d 248, 252–53 (C.C.P.A. 1963).

275. *See* Freilich, *supra* note 24, at 1, 3, 5 (defining fictional experiments in patent specifications as "prophetic examples"; stating that the USPTO allows for "fictional" data in a patent specifications, but has never explicitly stated its reasons for doing so).

276. *See* Seymore, *Uninformative Patents*, *supra* note 96, at 390–91 (suggesting that complex inventions in the unpredictable arts are opaque with respect to the inner workings and that inventions have become opaquer over time.).

277. *See* Freilich, *supra* note 24, at 1.

278. *See* Ewing, *supra* note 129, at 676.

279. *See* Furukawa et al., *supra* note 167, at 974–75; Gowers et al., *supra* note 169, at 309–10.

> identified over 300 MOFs with a predicted methane-storage capacity better than that of any known material, and this approach also revealed structure-property relationships. Methyl-functionalized MOFs were frequently top performers, so we selected one such promising MOF and experimentally confirmed its predicted capacity.[280]

This quote from a computational research study gives an example of *hypothetical* structures that may be fictional.[281] Should US patent law allow for the use of computational research capabilities for meeting the substantial and specific utility requirement with *hypothetical* chemical structures[282] in prophetic examples and patent specification that provides fictional data?[283] Early disclosure of underdeveloped inventions enabled by computational capabilities in the unpredictable arts tips the policy scale too far. Instead of allowing researchers to utilize computational research capabilities to prophesize and file patent claims of possibilities, US patent law should evolve to require a showing of some semblance of synthetic experiments, even if just a plan for physical experimentation.

A requirement of a laboratory-based working example, as proposed herein, would provide an appropriate balance between permitting early disclosure and satisfying the current standard of substantial and specific utility.[284] The proposed laboratory-based working example would enable inventors to hypothesize roadmaps for future research,[285] without carrying out any experiments in reduction to practice. For example, a laboratory-based working example would require demonstrating some coupling to equipment, whereas in current US patent law, actual reduction to practice would require sufficient testing or making of a product.[286] While reducing this burden on the inventor, a laboratory-based working example would retain the presumption of utility being met at the time of filing the patent application[287] and shift the burden on the patent applicant when the patent examiner had made a prima facie case of utility not being met.[288]

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280. Christopher E. Wilmer et al., *Large-Scale Screening of Hypothetical Metal-Organic Frameworks*, 4 NATURE CHEMISTRY 83, 83 (2012).

281. *See* Freilich, *supra* note 24, at 1.

282. *See* Coudert & Fuchs, *supra* note 175, at 211; Maurin, *supra* note 238, at 208, 210.

283. *See* Freilich, *supra* note 24, at 1, 3, 5.

284. *See* Seymore, *Patently Impossible*, *supra* note 99, at 190–91, 201, 206–07.

285. *See* Freilich, *supra* note 24, at 1.

286. *See* MPEP, *supra* note 13, § 2138.05, (defining actual reduction to practice as requiring testing, for which its nature depends on the particular facts of a case and the invention, and making of a product where the invention is more than a method).

287. *See* Seymore, *Presumption of Patentability*, *supra* note 83, at 995.

288. *Id.* at 998.

Unlike another proposal to provide any type of working example only upon request by a patent examiner,[289] this proposal would require a laboratory-based working example, which must be coupled to laboratory-based physical or tangible items. A laboratory-based working examples, as described herein, are apparatuses, chemicals, consumables, equipment, hardware, instrumentation, measurement tools, reagents, or physical or tangible items that can support or validate a computational research hypothesis in the unpredictable arts. These working examples are not captured in the third *Wands* factor, which assesses enablement (not utility), and considers "the presence or absence of working examples" [290] without specifying the types of working examples—thus leaving it to a patent examiner or a judge to evaluate the scope of working example.

Computationally derived inventions should provide a laboratory-based working example in the patent specification to demonstrate utility at the time of filing a patent application. Thus, for example, a laboratory-based working example can be shown in a patent specification as a diagram or drawing, or can be explained in conjunction with a description of a computational technique. The laboratory-based working example would couple computational capabilities with a working, tangible structure utilized in a laboratory. In doing so, the laboratory-based working example would demonstrate coupling prophesies to near experimental plans. In effect, such working examples would demonstrate more than just a prophesy[291] or a genus patent claim[292] of a family of hypothetical compounds, and more than incredible utility.[293] Rather, a laboratory-based working example would address a major doctrinal shortcoming in utility doctrine, in light of advancements in computational technologies, by modulating the utility standard slightly towards an experimental plan without requiring experiments to be conducted. An inventor's description of the potential use of a laboratory-based working example in the specification of a patent application at the time of filing would enable US patent law to evolve in response to the advent, adoption, and proliferation of computational research in the unpredictable arts.[294]

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289. Sean B. Seymore, *The Teaching Function of Patents*, 85 NOTRE DAME L. REV. 621, 631, 641–43, 645–46 (2010) [hereinafter Seymore, *Teaching Function of Patents*] (proposing a working example). However, this proposal does not mention being affiliated with a laboratory setting.

290. *See In re* Wands, 858 F.2d 731, 737 (Fed. Cir. 1988).

291. *See* Holbrook, *supra* note 22, at 157–58.

292. *See* MPEP, *supra* note 13, § 806.04.

293. *See In re* Citron, 325 F.2d 248, 253 (C.C.P.A. 1963).

294. *See* Seymore, *Heightened Enablement*, *supra* note 1, at 144, 155.

1. Implementation in Representative Computational Applications

A laboratory-based working example can address the shortcomings of the utility doctrine with GCMC simulations,[295] as well as the shortcomings of the enablement doctrine with computationally created chemical intermediaries.[296] The computation application examples in this Article have demonstrated that early patent filings have drawbacks,[297] which can be addressed with a laboratory-based working example at the time of filing a patent application.

First, to illustrate the implementation of a laboratory-based working example, consider its application to GCMC simulations of MOFs.[298] Suppose that a computational researcher has utilized GCMC methods to simulate hundreds of thousands of hypothetical MOFs with high-precision prediction of properties[299] that are described in a patent specification and claimed in patent claims. Rather than spending a patent examiner's time and the USPTO's resources in evaluating whether patentability requirements are met from a computationally derived invention, the use or indication of a laboratory-based working example would allow the computational researcher patent applicant to demonstrate a substantial and specific utility[300] at the time of filing the patent application. Unlike another proposal, which requires that a patent examiner make a prima facie utility rejection, request a working example of some sort when the written description is inadequate, and leave it to the examiner to enter the applicant's amendment,[301] this Article's proposal requires the patent applicant to demonstrate a laboratory-based working example coupling the simulated, hypothetical MOFs to laboratory-based, working tangible items at the time of filing the patent application. As an example, the patent applicant can provide tangible, laboratory-based items for MOF preparation as a diagram, drawing, or in the patent specification,[302] such as a water harvester for driving off water vapor from MOFs,[303] ultrasound equipment for rapid

295. *See supra* Section IV.A.2.

296. *See supra* Section IV.B.2.

297. *See* Seymore, *Teaching Function of Patents*, *supra* note 289, at 658–61 (arguing that ex ante incentives that encourage early filing can thwart innovation).

298. *See supra* Section IV.A.2.

299. *See* Coudert & Fuchs, *supra* note 186, at 211; Gowers et al., *supra* note 180, at 309–10; Maurin, *supra* note 238, at 208, 210; Wilmer et al., *supra* note 280, at 83; Xie et al., *supra* note 185, at 1.

300. *See* Seymore, *Serendipity*, *supra* note 5, at 208–209.

301. *See* Seymore, *Teaching Function of Patents*, *supra* note 289, at 641–43.

302. Dey et al., *supra* note 168, at 6.

303. Robert Sanders, *Device Pulls Water from Dry Air, Powered Only by the Sun*, BERKELEY NEWS (Apr. 13, 2017), http://news.berkeley.edu/2017/04/13/device-pulls-water-from-dry-air-powered-only-by-the-sun/ [https://perma.cc/3D9L-MLZS].

MOF synthesis under solvent-free conditions,[304] or a sealed reactor for removing unreacted starting materials.[305]

Second, to illustrate the implementation of a laboratory-based working example, consider its application to computationally created chemical intermediaries.[306] Suppose that a computational researcher has utilized machine learning methods to generate a library of chemicals and reactions to yield chemical intermediaries.[307] This Article's proposal requires the patent applicant to provide a laboratory-based working example demonstrating coupling of the computationally-created intermediaries. As an example, the patent applicant can provide tangible laboratory-based items as a diagram, drawing, or in the patent specification, such as lab ovens, furnaces, instruments, or centrifuges[308] to couple the computationally created intermediaries to plans for experiments.

2. Response to Critique of Laboratory-Based Working Example

Although a laboratory-based working example would provide a solution to the problem of subsuming the enablement requirement into the utility requirement for computationally derived inventions, competing policy considerations explain why Congress and courts have resisted making such a change. The primary concern is that it would require the patent applicant to engage in additional prefiling activities. The effect could be a delay to filing a patent application, which could compromise patent rights in the United States and internationally, thus potentially enabling a competitor with greater resources to file a timelier patent application. A secondary concern is that requiring a laboratory-based working example would create a narrower patent right, which may discourage inventors pursuing patent protection. The effect could be an increase in trade secret protection,[309] or if inventors

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304. *Ultrasonic Preparation of Metal-Organic Frameworks (MOFs)*, HIELSCHER ULTRASOUND TECH., https://www.hielscher.com/ultrasonic-preparation-of-metal-organic-frameworks-mofs.htm [https://perma.cc/HCW6-4WZR] (last visited Jan. 28, 2019).

305. Atanu Kumar Das et al., *An Efficient Synthesis Strategy for Metal-Organic Frameworks: Dry-Gel Synthesis of MOF-74 Framework with High Yield and Improved Performance*, 6 SCI. REP. 1, 2 (2016).

306. *See supra* Section IV.B.2.

307. *See supra* Section IV.B.2.

308. *LAB EQUIPMENT*, THERMOFISHER SCI., https://www.thermofisher.com/us/en/home/life-science/lab-equipment.html [https://perma.cc/QU5P-45PT] (last visited Jan. 28, 2019).

309. *See* Kewanee Oil Co. v. Bicron Corp., 416 U.S. 470, 481–485 (1974) (specifying that trade secret law also encourages research and development in stating, "[t]rade secret law will encourage invention in areas where patent law does not reach, and will prompt the independent innovator to proceed with the discovery and exploitation of his invention . . ." and that "[c]ompetition is fostered and the public is not deprived of the use of valuable, if not quite patentable, invention"); Risch, *supra* note 245, at 11, 38, 43.

do choose patent protection, then competitors and imitators could more easily develop design-around strategies[310] over a filed patent application.

In response to each of these critiques, it is important to recognize that the current utility requirement itself could impede innovation. Specifically, an overly broad utility standard could dominate an entire technology field and thereby prevent other inventors in the field from pursuing related inventive activity.[311] Moreover, the current utility standard could allow for the use of computational capabilities to help capture entire families of chemical compounds for defensive patenting to extinguish others' potential patent rights.[312]

The current allowance of prophetic examples[313] enabled by computational capabilities would dominate other technological innovations by subsequent inventors in the field. The use of computational capabilities to capture, for example, GCMC simulations of hundreds of thousands of MOFs or crucial computationally created chemical intermediaries in patent claims would "diminish . . . potential rewards as incentive to invent and would thus discourage [subsequent inventors'] creative efforts."[314] The utility standard in US patent law should be strengthened with a laboratory-based working example in order to "promote the flow of information about inventions from patentees to potential future innovators, thereby stimulating increased and speedier follow-up innovation."[315]

Moreover, the additional requirement of a laboratory-based working example would reduce uncertainty within the unpredictable arts.[316] If this initial utility-related coupling of computational capabilities with laboratory-based tangible items is disclosed at an early stage of research and development, it also reduces uncertainty

310. Shyla Shirodkar, *Design-Around Patent Strategies for Patentees and Competitors* , 5 L.J. NEWSLS. 1, 1 (2004).

311. M. Sharon Webb, *Patent Pitfalls for Early Stage Investors*, 5 VENTURE CAP. J. 1, 2 (2004), https://www.goodwinlaw.com/~/media/Files/Publications/Attorney%20Articles/2004/Patent_Pitfalls_for_Early_Stage_Investors.pdf [https://perma.cc/K9FU-EAUC].

312. Bill Barrett, *Defensive Use of Publications in an Intellectual Property Strategy*, NATURE PUBL'G GRP. (2002), https://www.nature.com/bioent/2003/030101/full/nbt0202-191.html [https://perma.cc/Y2KV-ZHQX] (suggesting that with defensive patenting, in disclosing an invention to the public, the patent applicant has nothing new to disclose to the public because the invention has already been disclosed, and therefore is already possessed by the public).

313. *See* Freilich, *supra* note 24, at 1.

314. *See* Richard H. Stern, *Solving the Algorithm Conundrum: After 1994 in the Federal Circuit Patent Law Needs a Radical Algorithmectomy*, 22 AIPLA Q.J. 167, 172 (1994); Consol. Elec. Light Co. v. McKeesport Light Co., 159 U.S. 465, 476 (1895) (explaining that overbreadth "operate[s] rather to discourage than to promote invention.").

315. Jeanne C. Fromer, *Patent Disclosure*, 94 IOWA L. REV. 539, 599 (2009).

316. *See* Seymore, *Heightened Enablement*, *supra* note 1, at 137–38, 144–45.

during the patent examination stage. A coupling of the computationally derived capability to a laboratory-based working example would also bolster enablement. A requirement of a laboratory-based working example at the time of filing a patent application would also have a post patent-issuance benefit with more clarity of licensing involving the patent.

B. Changing Patent Examiner Hiring and Training in the Unpredictable Arts

The implementation of a laboratory-based working example would strengthen the utility requirement in US patent law. However, inventors may simply provide diagrams or figures of tangible, laboratory-based items in the patent specification in hopes of satisfying this proposed heightened requirement. A patent applicant can utilize computational capabilities[317] to develop hypothetical chemical compounds to file prophetic examples and simply provide a diagram or figure of a tangible, laboratory-based item in hopes that the patent examiner will not make a rejection based on the proposed laboratory-based working example requirement. One reason that a patent applicant utilizing computational capabilities can overcome a heightened utility requirement is that patent examination lacks an understanding of computational experimentation. As an example, suppose the following scenario:

> [An inventor and patent applicant] could . . . generate millions upon millions of plausible chemical structures and load them into multiple patent applications together with one compound that actually meets all of the patentability [requirements] in each patent application. The applicant could then claim that enabled compound and get a patent issued on the compound and have the rest of the [disclosed but unclaimed] structures become enabled prior art . . . .[318]

In this example, the patent applicant has utilized computational capabilities to generate millions of hypothetical chemical compounds, with one compound in each patent application meeting patentability. The patent applicant has engaged in a defensive patenting strategy[319] in an attempt to use the non-enabled, disclosed chemical compounds to serve as prior art and block other subsequent inventors from patenting the non-enabled chemical compounds. Thus, the weak or unclear utility requirement would allow a computationally derived chemical compound meeting patentability to block others' subsequent inventions.

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317. *See supra* Sections IV.A.2, IV.B.2.

318. CHRIS P. MILLER & MARK J. EVANS, THE CHEMIST'S COMPANION GUIDE TO PATENT LAW 170 n.4 (2010).

319. *See* Barrett, *supra* note 312.

A heightened utility requirement of a laboratory-based working example would be one mechanism to prevent such defensive patenting,[320] since it would strengthen the utility requirement for one particular compound in each patent application attempting to meet patentability.

Besides strengthening the utility requirement for the patent applicant, another strategy to prevent such blocking tactics is to bolster capabilities in patent examination. For example, patent examination improvements could allow an examiner to better detect whether the proposed laboratory-based working example utility requirement would be coupled to hypothetical chemical structures in the patent claims and detailed description of the patent specification. In other words, patent examination capabilities are needed to discern whether the proposed laboratory-based working example in a diagram or figure is adequately described in the detailed description to show that the patent applicant has thought of some semblance of an experimental plan for synthesizing the hypothetical chemical compounds.

One mechanism to improve patent examination is to change patent examiner hiring norms and patent examiner training in the unpredictable arts. The current practice of hiring patent examiners is based on specific educational backgrounds and degrees[321] and ignores computational degree programs.[322] USPTO hiring announcements specify job description requirements[323] indicating expertise in specific

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320. *See id.*

321. *See Job Announcement – Patent Examiner (Chemical, Mechanical, or Electrical)*, USA JOBS, https://www.usajobs.gov/GetJob/ViewDetails/506671000 [https://perma.cc/H99T-NNBQ] (last visited Jan. 28, 2019) (showing many vacancies for a patent examiner position requiring either a chemical, mechanical, or electrical engineering background); *Job Announcement – Patent Examiner (Electrical Engineer)*, USA JOBS, https://www.usajobs.gov/GetJob/PrintPreview/490728500 [https://perma.cc/L2W2-P7B3] (last visited Jan. 28, 2019) (specifying a patent examiner job requiring an electrical engineering background); *Job Announcement Now Open for Patent Examiners (2017)*, U.S. PAT. & TRADE OFF., https://www.uspto.gov/sites/default/files/documents/Examiner%20brochure%202017.pd [https://perma.cc/GZ7Y-E2TW] (last visited Jan. 28, 2019) (specifying that the Basic Qualification are "Minimum of Bachelor's degree in engineering or science," without any mention of any computational education or experience).

322. *See Graduate and Undergraduate Programs in Computational Science*, SOC'Y INDUS. & APPLIED MATHEMATICS, https://www.siam.org/Students-Education/Resources/For-Graduate-Students/Detail/graduate-and-undergraduate-programs-in-computational-science [https://perma.cc/3LWB-E7E5] (last visited Jan. 15, 2019); *We're Hiring! Patent Examiner Information Session – Webcast*, U.S. PAT. & TRADEMARK OFF., https://www.uspto.gov/about-us/uspto-locations/silicon-valley-ca/we-re-hiring-patent-examiner-information-session [https://perma.cc/WTH3-8VUB]. *See generally Job Announcement – Patent Examiner (Electrical Engineer)*, *supra* note 321.

323. *See* Lisa Parmley, *Complete Guide to a Career as a Patent Examiner*, PAT. EDUC. SERIES (Feb. 1, 2018), https://www.patenteducationseries.com/patent-career/patent-examiner-career.html [https://perma.cc/2VYR-XWJ5] (indicating that the job description of a patent examiner calls for ensuring patent applications conform to requirements, investigating whether

technology areas,[324] such as electrical, or computer, or mechanical,[325] but lack any reference to computational education or experience.[326]

Patent examiner training is similarly tied to employment in a particular technology center.[327] After being hired into that technology area, a patent examiner's subject matter training is aligned with the scope of coverage required to assess patents assigned to that technology center. Since a patent examiners' performance measurement is largely based on productivity,[328] the USPTO provides patent examiners training to make their tasks[329] more productive.[330] Thus, training for

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an invention is described clearly and used appropriately, undertaking manual searches of earlier publications to establish novelty of an invention, considering technical issues related to an invention, producing search reports and sending them to applicants, and acting as a liaison between applicants in matters of dispute resolution).

324. *See Patent Technology Centers Management*, U.S. PAT. & TRADE OFF., https://www.uspto.gov/patent/contact-patents/patent-technology-centers-management [https://perma.cc/P7FN-DBWV] (last visited Jan. 15, 2019).

325. *See We're Hiring! Patent Examiner Information Session – Webcast*, *supra* note 322.

326. *See #USPTOJobsHQ16: Patent Examiner Career Open House*, U.S. PAT. & TRADEMARK OFF., https://www.uspto.gov/jobs/usptojobshq16-patent-examiner-career-open-house [https://perma.cc/HQ26-NNQX] (last visited Feb. 9, 2019); Parmley, *supra* note 323.

327. *See* Gary Welch & Bao-Thuy Nguyen, Office of Patent Training, Presentation for the U.S. Patent & Trade Office: Patent Quality Chat: Training for the Examination of High Quality Patents 15–19 (Mar. 16, 2017), https://www.uspto.gov/sites/default/files/documents/Patent%20Quality%20Chat%20March%202017%20Final%20for%20presentation.pdf [https://perma.cc/T8NT-32Q4] (showing Patent Examiner Technical Training Program seminars, in which experts from industry and academia participate as guest lecturers to provide technical training and expertise to patent examiners regarding the state of the art at tech fairs based on classification of a patent examiner in a particular technology center, such as: 1600 for Biotechnology & Organic Chemistry; 1700 for Chemical & Material Engineering; 2100 Computer Architecture & Software; 2400 for Networking, Multiplexing, Cable & Security; 2600 for Communications; 2800 for Semiconductors, Memory, Optics, Photocopying, Electrical Circuits & Systems, Printing, Measuring & Testing; 2900 for Design Day; 3600 for Transportation, Construction, Electronic Commerce, Agriculture, and National Security; 3700 for Mechanical, Medical Device Customer Partnership & Gaming Technologies.

328. *See* Naira Rezende Simmons, *Putting Yourself in the Shoes of a Patent Examiner: Overview of the United States Patent and Trademark Office (USPTO) Patent Examiner Production (Count) System*, 17 J. MARSHALL REV. INTELL. PROP. L. 32, 32–33, 41 (2017) (describing that under the current production system, productivity is assessed based on Production Units ("PUS") achieved relative to the Examiner's production goal, which is calculated based on the number of "Examining Hours" and on different "counts"; providing that a patent examiner's tasks include "reading and understanding patent specifications, searching the prior art to determine what technological contribution the application teaches the public, and evaluating the scope of the claims").

329. *See* Parmley, *supra* note 323 (specifying that the role of a patent examiner is to issue valid patents and to act as the public's advocate, including making appropriate rejections and reasonable rejections to patent applications).

330. *See* U.S. PAT. & TRADEMARK OFF., PERFORMANCE & ACCOUNTABILITY REPORT 2017, at 162 (2017); Simmons, *supra* note 328, at 36 (describing that a patent examiner's productivity is assessed based on the number of hours that patent examiners at different grade level are allotted to spend on each patent application).

patent examiners is coupled to their technical or science education and employment in a particular technology center.[331]

The USPTO should introduce computational education and skills in its hiring norms and training for patent examiners. First, the USPTO should consider undergraduate and graduate degrees in computational science, computational engineering, or similar computational disciplines[332] as an education qualification in its hiring requirements and promote such computational education in its hiring announcements. Second, the USPTO should implement computational science or computational engineering subject matter content into its patent examiner training efforts, such as its Examination Guidance and Training Materials,[333] Patent Examination Technical Training Program,[334] Site Experience Education Program,[335] and Stakeholder Training on Examination Practice and Procedure.[336] In order to improve the assessment of patentability requirements, the USPTO should hire and train patent examiners on computational experimentation to better assess patentability in the unpredictable arts. Since computational capabilities are proliferating among inventors in unpredictable arts, the USPTO needs to develop an understanding of computational capabilities among its patent examiners. As more scientists and engineers conduct research in the unpredictable arts involving computational capabilities, patent examiners will increasingly need to possess similar computational skills to complete their tasks and assess computationally derived inventions.

1. Implementing Computational Backgrounds and Training for Patent Examination

Many art units could benefit from having personnel possessing computational training. The hiring and training proposal of

331. *See* Parmley, *supra* note 323; *Office of Patent Training*, U.S. PAT. & TRADEMARK OFF., https://www.uspto.gov/patent/office-patent-training#step2 [https://perma.cc/43B5-C5BG] (last visited Jan. 17, 2019); *Patent Technology Centers Management*, *supra* note 324.

332. *Graduate and Undergraduate Programs in Computational Science*, *supra* note 322.

333. EXAMINATION GUIDANCE AND TRAINING MATERIALS, *supra* note 269.

334. *Patent Examiner Technical Training Program*, U.S. PAT. & TRADEMARK OFF., https://www.uspto.gov/patent/initiatives/patent-examiner-technical-training-program-pettp-0#step2 [https://perma.cc/4R3Q-LVR5] (last visited Jan. 16, 2019).

335. *Site Experience Education (SEE) Program*, U.S. PAT. & TRADEMARK OFF., https://www.uspto.gov/patent/initiatives/site-experience-education-see-program [https://perma.cc/693Y-FACD] (last visited Jan. 16, 2019).

336. *Stakeholder Training on Examination Practice and Procedure (STEPP)*, U.S. PAT. & TRADEMARK OFF., https://www.uspto.gov/patent/initiatives/stakeholder-training-examination-practice-and-procedure-stepp [https://perma.cc/P7E3-7ZDJ] (last visited Jan. 16, 2019).

computational backgrounds for patent examiners should be implemented in the USPTO's Technology Center 1600 and Technology Center 1700, each of which examines patent applications in the unpredictable arts. Technology Center 1600 provides examination for patent application concerning biotechnology and organic fields and Technology Center 1700 provides examination for patent applications including chemistry and materials engineering fields.[337] Technology Center 1600's examination of patent applications in arts units 1611-1619, 1621-1629, 1631-1639, 1642-1649, 1651-1658, and 1661-1663[338] are particularly probable recipients of patent applications of computationally derived inventions of organic compounds. Technology Center 1700's examination of patent applications in art units 1760, 1710, and 1730[339] are also particularly probable recipients of patent applications of computationally derived inventions of organic chemistry, polymers, and chemistry.

These art units in Technology Center 1600 and Technology Center 1700 should implement hiring practices that accept graduates of degree programs in computational science, computational engineering, or other similar computational disciplines.[340] These art units in Technology Center 1600 and Technology Center 1700 should proactively find and bring computational science and engineering professors and researchers from universities and industrial research laboratories to the Patent Examiner Technical Training Program Technology Fairs.[341] The UPSTO patent examination guidance and training materials—which lack any materials concerning examination for utility[342]—should be updated to reflect best practices, examples, guidance, and training of computationally derived inventions towards meeting the utility requirement for patentability. Any such updates to

337. *Patent Technology Centers Management*, *supra* note 324.

338. *TC 1600 Management Roster*, U.S. PAT. & TRADEMARK OFF., https://www.uspto.gov/patent/contact-patents/tc-1600-management-roster [https://perma.cc/9YKL-QKRL] (last visited Jan. 16, 2019) (providing descriptions of arts units in 1611-1619 as belonging to "1610 Organic Compounds: Bio-affecting, Body Treating, Drug Delivery, Steroids, Herbicides, Pesticides, Cosmetics, and Drugs"; art units in 1621-1629 as belonging to "1620 Organic Chemistry"; art units 1631-1639 as belonging to "1630 Molecular Biology, Bioinformatics, Nucleic Acids, Recombinant DNA and RNA, Gene Regulation, Nucleic Acid Amplification, Animals and Plants, Combinatorial/Computational Chemistry").

339. *TC 1700 Management Roster*, U.S. PAT. & TRADEMARK OFF., https://www.uspto.gov/patent/contact-patents/tc-1700-management-roster [https://perma.cc/8UNA-6A5L] (last visited Jan. 16, 2019) (providing descriptions of arts units in 1760 as comprising "Organic Chemistry, Polymers, and Compositions"; 1710 as comprising "Coating, Etching, Cleaning, [and] Single Crystal Growth"; 1730 as comprising "Metallurgy, Metal Working, Inorganic Chemistry, Catalysts, Electrophotography, [and] Photolithography").

340. *Graduate and Undergraduate Programs in Computational Science*, *supra* note 322.

341. *See Patent Examiner Technical Training Program*, *supra* note 334.

342. *See* EXAMINATION GUIDANCE AND TRAINING MATERIALS, *supra* note 301.

the UPSTO patent examination guidance and training materials should introduce the proposed laboratory-based working example to asses utility.[343]

2. Response to Critique of Patent Examination Hiring and Training

Criticism to changes in hiring norms and training of patent examiners in response to computationally derived inventions center on the USPTO's resources. The USPTO is an administrative agency of the US Department of Commerce[344] that is responsible for maintaining its own finances.[345] Critiques of the proposed hiring and training reforms may point out that patent examiners are at capacity for evaluating patent applications[346] and that changes to hiring or training may have deleterious effects on the USPTO and its backlog of pending patent applications.[347]

It is important to recognize that the current patent examination itself could impede innovation. Specifically, outdated patent examination in Technology Center 1600 and Technology Center 1700 could result in allowing into the patent system computationally derived patent applications for which patent examiners lack necessary interpretation skills. Since patent examiners must be adept at new aspects of technology,[348] art units in the unpredictable arts must employ and train patent examiners with computational backgrounds. Thus, even if patent examiners are overburdened,[349] training patent

343. *See supra* Section V.A.

344. U.S. DEP'T COMMERCE, STRATEGIC PLAN 2018–2022, at 2 (2018), https://www.commerce.gov/sites/default/files/us_department_of_commerce_2018-2022_strategic_plan.pdf [https://perma.cc/K5FZ-JJCG]; *Bureaus and Offices*, U.S. DEP'T COMMERCE, https://www.commerce.gov/bureaus-and-offices [https://perma.cc/4U8P-S8PD] (last visited Jan. 16, 2019).

345. *Budget and Financial Information*, U.S. PAT. & TRADEMARK OFF., https://www.uspto.gov/about-us/performance-and-planning/budget-and-financial-information [https://perma.cc/2ARS-LMQG] (last visited Jan. 16, 2019).

346. Jeffrey M. Kuhn, *Information Overload at the U.S. Patent and Trademark Office: Reframing the Duty of Disclosure in Patent Law as a Search and Filter Problem*, 13 YALE J.L. & TECH. 90, 92 (2010–2011).

347. Ayal Sharon & Yifan Liu, *Improving Patent Examination Efficiency and Quality: An Operations Research Analysis of the USPTO, Using Queuing Theory*, 17 FED. CIR. B.J. 133, 133 (2008).

348. *See* Simmons, *supra* note 328, at 33.

349. *See* Kuhn, *supra* note 346, at 92.

examiners with computational expertise will yield higher quality patents[350] and lead to less downstream patent litigation.[351]

The current hiring norm of seeking and employing patent examiners with noncomputational degree programs, such as chemical, computer, electrical, or mechanical engineering disciplines,[352] ignores the necessary expertise for evaluating computationally derived inventions. While fundamentals of chemistry, mathematics, and physics are necessary for computational degree programs,[353] computationally trained scientists and engineers are adept in advanced subjects involving computer science, mathematics, numerical analysis, simulation and modeling, and statistics.[354] Patent examiners who have graduated from the traditional degree programs sought by the art units in the unpredictable arts lack the skills to assess computationally derived inventions. While it would be preferable to hire patent examiners who are graduates from computational degree programs, some computational skills can be taught to patent examiners by computational science and engineering professors and researchers from universities and industrial research laboratories through training.[355]

C. Innovation Policy Considerations for Computational Reform Proposals

The disclosure function of patents promotes innovation through dissemination of information about inventions.[356] There are innovation implications of how early to grant patent protection[357] and the necessary disclosure needed at the early stages of an invention. The prospect theory of patent law suggests that granting broad patent

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350. *See* Eric D. Blatt & Lian Huang, *Do Heightened Quality Incentives Improve the Quality of Patentability Decisions?: An Analysis of Trend Divergences During the Signatory Authority Review Program*, 46 AIPLA Q.J. 162, 167 (2018) (suggesting that patent examiners may respond to heightened patentability requirements and heightened patent quality requirements by increasing the quality of their patentability decisions).

351. *See* Matthew John Duane, *Lending a Hand: The Need for Public Participation in Patent Examination and Beyond*, 7 CHI.-KENT J. INTELL. PROP. 57, 68 (2008).

352. *See* sources cited *supra* note 321.

353. *SIAM Working Group on CSE Education*, SOC'Y INDUS. & APPLIED MATHEMATICS, https://www.siam.org/Students-Education/Resources/For-Graduate-Students/Detail/research-and-education-in-computational-science-and-engineering [https://perma.cc/B3J9-FQHK] (last visited Jan. 16, 2019) (specifying that computational application areas require a basic knowledge of courses in chemistry, mathematics, and physics).

354. *See* Ulrich Rüde et al., *Research and Education in Computational Science and Engineering*, 60 SIAM REV. 707, 740–41 (2018).

355. *Patent Examiner Technical Training Program*, *supra* note 334.

356. Seymore, *Uninformative Patents*, *supra* note 96, at 395–96.

357. *See* Rebecca S. Eisenberg, *Analyze This: A Law and Economics Agenda for the Patent System*, 53 VAND. L. REV. 2081, 2087–88 (2000).

rights in early stages of innovation will promote efficiency in the further development of related, promising technological prospects.[358] However, granting too-early patent rights could create blocking patents and have chilling effects that burden society by preventing follow-on inventions.[359]

The advent, adoption, and proliferation of computational research capabilities[360] in the unpredictable arts allows inventors to seek patent protection in early stages of their research and development. The proposed computational reforms of a laboratory-based working example[361] and changes in patent examiner hiring norms and training[362] modulate the gatekeeping patentability requirements of enablement and utility to become more strong and clear. The ability of inventors to experiment with properties, structures, and reactions *in silico* requires that US patent law respond in order to discourage inventors from claiming subject matter that is purely hypothetical or too nascent. Rather than have patent applicants provide postfiling evidence,[363] a heightened utility requirement in an era of computational experimentation would better align with recent judicial efforts to tighten patentability standards.[364] Indeed, scholars have suggested that advancements in digitally-based, emerging technologies necessitate weakening patent rights,[365] which can be attained by strengthening by patentability requirements.

In effect, this Article's proposed computational reforms would create an innovation policy change with respect to certain classes of inventions in the unpredictable arts, namely drug compounds, materials, and pharmaceuticals. Society would benefit by preventing speculation and rewarding inventors for what effectively are guesses in

358. *See* Edmund W. Kitch, *The Nature and Function of the Patent System*, 20 J.L. & ECON. 265, 276 (1977).

359. *See* George C. Lewis, *The Cautionary Tale of Crocs and the New World of Instant Competition*, 37 COLO. LAW. 39, 41 (2008); Robert Merges, *Intellectual Property Rights and Bargaining Breakdown: The Case of Blocking Patents*, 62 TENN. L. REV. 75, 81 (1994).

360. *See supra* Part II.

361. *See supra* Section V.A.

362. *See supra* Section V.B.

363. *See* Holbrook, *supra* note 253, at 1487–88; Holger Tostmann, *Protecting Chemistry Inventions: The Double-Edged Sword of Being an Unpredictable Art*, 6 ACS MED. CHEMISTRY LETTERS 364, 364 (2015) (noting that data collected at a later stage of research and development could further support data shown in the already-filed patent application).

364. Seymore, *Foresight Bias*, *supra* note 73, at 1106.

365. Mark A. Lemley, *IP in a World Without Scarcity*, 90 N.Y.U. L. REV. 460, 464 (2015) (suggesting that the development of cost-reducing technologies weakens the case for intellectual property law protections); Lucas S. Osborn, Joshua M. Pearce & Amberlee Haselhuhn, *A Case for Weakening Patent Rights*, 89 ST. JOHN'S L. REV. 1185, 1189–90 (2015) (suggesting that emerging technologies that reduce the research, development, and commercialization costs should decrease the relative need for the patent system and therefore, patent should be significantly weakened).

those fields of research. Another innovation policy consideration is that the proposed computational reforms could push inventors towards trade secret protection[366] if securing patent protection becomes more arduous, costly, or time consuming. A lack of clarity for patentability would motivate researchers to seek cheaper protection through cheaper measures, such as trade secret law.[367] Also, greater expense in attempting to achieve patentability with a longer patent prosecution timeline could push researchers to pursue patent and trade secret complementary protection as an alternative to patent protection alone, and in doing so, produce socially harmful results.[368] Indeed, society would better benefit from this Article's proposal to require patent application disclosures that demonstrate some semblance of experimental planning and can be adequately examined by computationally qualified patent examiners.

VI. CONCLUSION

Computational research capabilities allow researchers and inventors to simulate chemical structures and compounds in advance of or in conjunction with synthesis. Science and engineering researchers are no longer limited to physical experiments for research and development; rather, researchers can utilize computation to experiment upon structure-activity relationships and predict properties of molecules and chemical reactions. It is no longer surprising that a researcher-inventor can simulate millions of hypothetical chemical compounds and prophetically claim a resulting broad genus without conducting a single physical experiment. While computational experimentation aids inventors in the conception process, it also weakens the scope of enablement and utility patentability requirements in US patent law. The result of the advent, adoption, and proliferation of computational capabilities is that enablement becomes subsumed into the utility doctrine. This doctrinal problem has become more acute as US patent law has been slow to respond. This Article

366. *See* Kewanee Oil Co. v. Bicron Corp., 416 U.S. 470, 485 (1974) ("Trade secret law will encourage invention in areas where patent law does not reach, and will prompt the independent innovator to proceed with the discovery and exploitation of his invention. Competition is fostered and the public is not deprived of the use of valuable, if not quite patentable, invention.").

367. *See* Risch, *supra* note 245, at 36, 38, 43 (2007) (discussing the economic value of trade secrecy, and pointing out that trade secret protection is achieved either by standard efforts to exclude and control or by non-standard precautions that are enhanced by fragmenting information).

368. *See* Simon & Sichelman, *supra* note 76, at 377, 379, 382 (contending that inventions that generate data about the invention that can be used to improve the invention itself can be maintained as a trade secret, but doing so would lead to anticompetitive and economically detrimental effects).

suggests that requiring a laboratory-based working example in the unpredictable arts would provide an appropriate balance between permitting early disclosure and satisfying the patentability requirements. In addition to strengthening the utility doctrine in response to computational experimentation, introducing computational education and skills in USPTO hiring norms and training for patent examiners would strengthen the detection and examination of computationally derived inventions. It is now time for US patent law to respond to computational experimentation. By reinvigorating patentability standards with a heightened utility requirement and modernizing patent examination in the unpredictable arts, innovation and society will benefit in a computational world.